# CONTAMINATION DES ALIMENTS EMBALLES

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# WHY ARE THEY SO INDISPENSABLE ?
# SHIFTING NEEDS ?












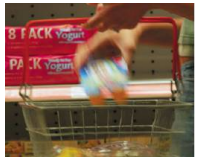




# SOURCES OF CONTAMINATION = PACKAGING MATERIALS

## CONTAMINANTS = PACKAGING SUBSTANCES (additives, monomers, residuals)


*Non food grade materials may be recycled with food grade materials.*

INRA

# Food and Feed Safety

English



## Food Contact Materials - Emerging Issues



The use of **recycled materials** and the design of **active and intelligent food packaging** are new trends. Active packaging is intended to extend the shelf life of the packaged food, while intelligent packaging monitors the conditions of packaged foods to give information about the quality of the food. Under review is how far these new packaging systems are covered by existing legislation and it amendments and/or new Directives are necessary to address these items.

The current approach for the authorisation and control of substances used in food contact materials is cautious in estimating the potential exposure of the consumer to these substances. Approaches which take better account of the actual **exposure of the consumer to food contact materials** in risk assessment are under discussion.

The use of **mathematical modelling** to predict migration, which can reduce the amount of tests to be undertaken, has been recently introduced into legislation. Practical examples for the application of this new concept are described in the "**Practical Guide.**" pdf

**ITX in babymilk** pdf

Standing Committee on the Food Chain and Animal Health, Section Toxicological Safety, **Conclusions** pdf of the meeting of 30 November 2005 with respect to the presence of isopropylthioxanthone (ITX) in milk for babies and other products.

**Commission statement on EFSA Opinion on ITX**

The European Commission has noted EFSA's advice of 9 December 2005 that the presence of ITX (2-Isopropylthioxanthone) in food, whilst undesirable, does not raise health concerns at the levels reported. ITX is a

**Resources**

- Speeches
- Press Releases
- Health & Consumer Voice Newsletter
- Publications
- Committees
- Links

**International Affairs**

- Organisations
- Codex
- Import Conditions
- Pets and Animal Welfare
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Food and Feed Safety

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Last Updated: Thursday, 16 October, 2003, 09:44 GMT 10:44 UK

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# Chemical found in baby food jars

**Baby food manufacturers have been urged to change the way they package their products amid fears over cancer.**

Many babies are given food from jars

The European Food Safety Authority says it has found traces of a potentially dangerous chemical in some jars.

Officials said there was no need for parents to stop giving their children food from jars because the cancer risk is extremely low.

However, they recommended that manufacturers consider introducing safer packaging.

## Cancer-causing chemical

The chemical, semicarbazide (SEM), has been found in very small quantities in some jars of food.

The authority said the chemical was not found in any particular type of food but rather food that was packaged in a specific way.

This included food sold in glass jars with metal lids, containing sealant gaskets.

> **"The risk to consumers resulting from the possible presence of semicarbazide in foods, if any, is judged to be very small"**
>
> Dr Sue Barlow,

The report says: "The foods that have been reported to contain SEM include baby foods, fruit juices,

WATCH AND LISTEN
**The BBC's Vicki Young**
"The risk is extremely small"
VIDEO

SEE ALSO:
- Fears over tuna health risk to babies
  17 Feb 03 | Health
- Baby food in tampering scare
  28 Aug 01 | UK
- Pesticide levels 'falling'
  07 Aug 02 | Health

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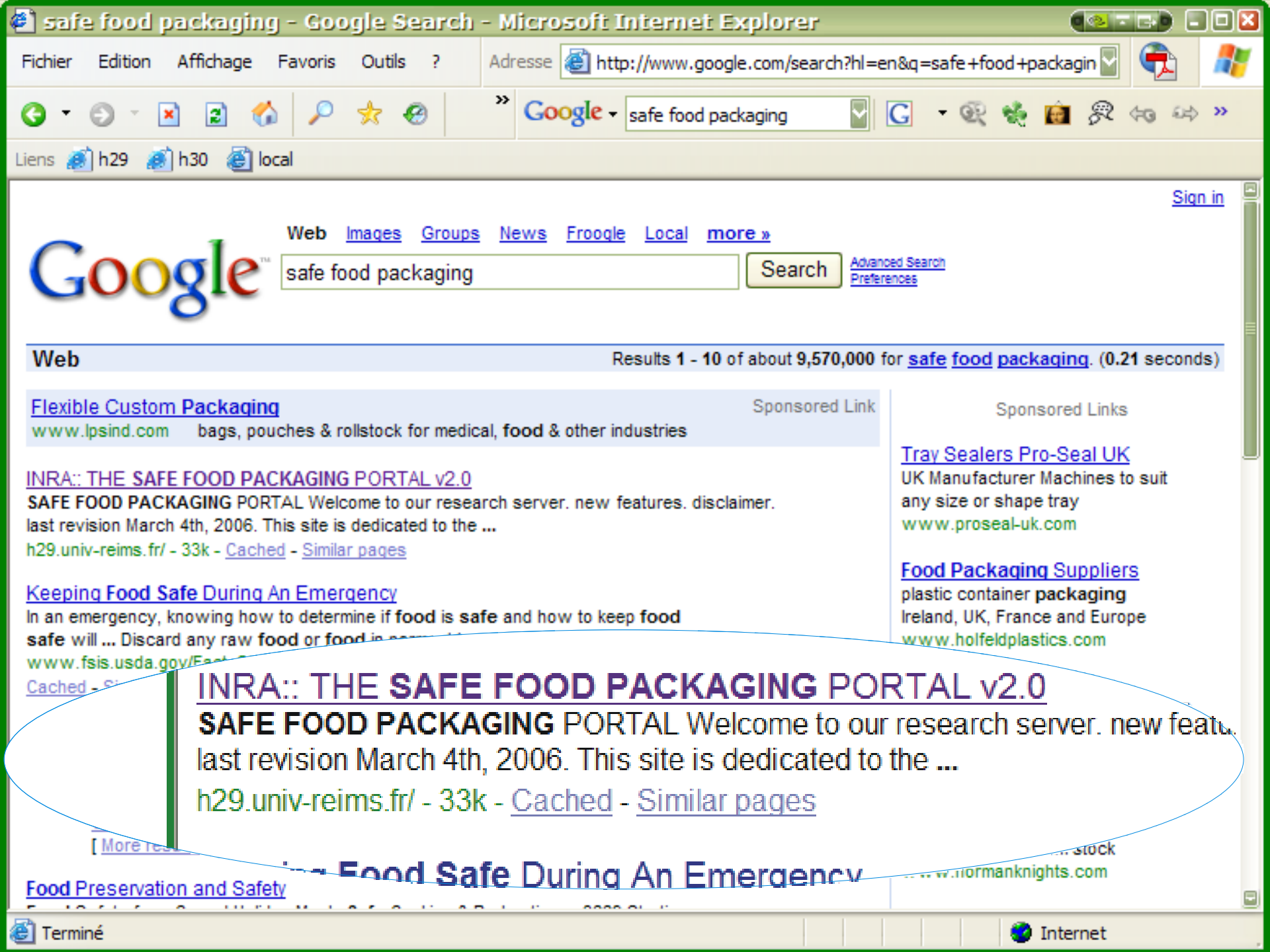
# RISK ISSUES

Risk = $f$ (perception, representation)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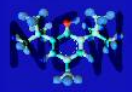

new features

# SAFE FOOD PACKAGING PORTAL

## Welcome to our research server

This site is dedicated to the developement of **decisions tools** based on *numerical simulation* and *databases* for the **food packaging** community.

The initial idea is to translate in a short way laboratory made computational tools into operative tools:

- for **compliance verification** according to the EU plastics directive 2002/72/EC,
- to optimize the design of **safe packaging** materials (with reduced migration),
- to assess the contamination level of packaged food available on the market (**risk assessment**),
- to contribute to the evaluation of the **consumer exposure** to substances orginating from plastic materials

*Click here to see some snapshots (the content depends on previous runs). Videos are freely available in the section "virtual experiments". Publications, which are relevant with the content of this site, are given here.*

**Visitors/users**, who are mainly interested in **COMPLIANCE TESTING** of food contact materials (FCM), are invited to follow first this link and to take a look at this webinar.

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**Functionalities which have been implemented via a web interface:**

- molecular calculations, 3D visualization, search of molecules
- decision trees,
- simulation of the diffusion in 1D and 2D (free geometry),
- recycled materials with functional barriers (with processing and storage considerations).

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**Current developements (testing phase) based on probabilistic simulation/modeling include:**

- MIGRARISK: modeling under uncertainties and variabilities (application to the risk of contamination of foodstuffs by susbstances originating from packaging materials),
- EXPORISK: exposure assessment at the scale of a group/pattern of consumers, households (for restricted users).

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Olivier Vitrac



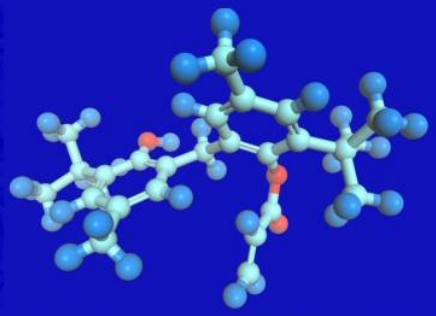
NEWS

**PhD position available**

research grant INRA-CNRS

Application deadline
31 March 2006

project description (English)
project description (French)
application form (French)
Grant description and conditions (French)



example of plastic additive (IRGANOX 3052)

LAST IMPROVEMENTS (non exhaustive)

- new databases (EaD, EaK, S, EaS), HTML code within database fields
- on line databases on D and K values
- multilayers improvements
- better communication between modules
- crossed links between pages
- advanced search of molecules
- fast preview of molecules
- some new videos
- presentation of Luigi Rossi (DG SANCO, EU Commission)

# 2 QUESTIONS VERROUS

**NOTRE DEMARCHE:** UTILISER NOS *CONNAISSANCES « PHYSICO-CHIMIQUES »* POUR EVALUER LE RISQUE DE CONTAMINATION DES ALIMENTS EMBALLES ET L'EXPOSITION DU CONSOMMATEUR

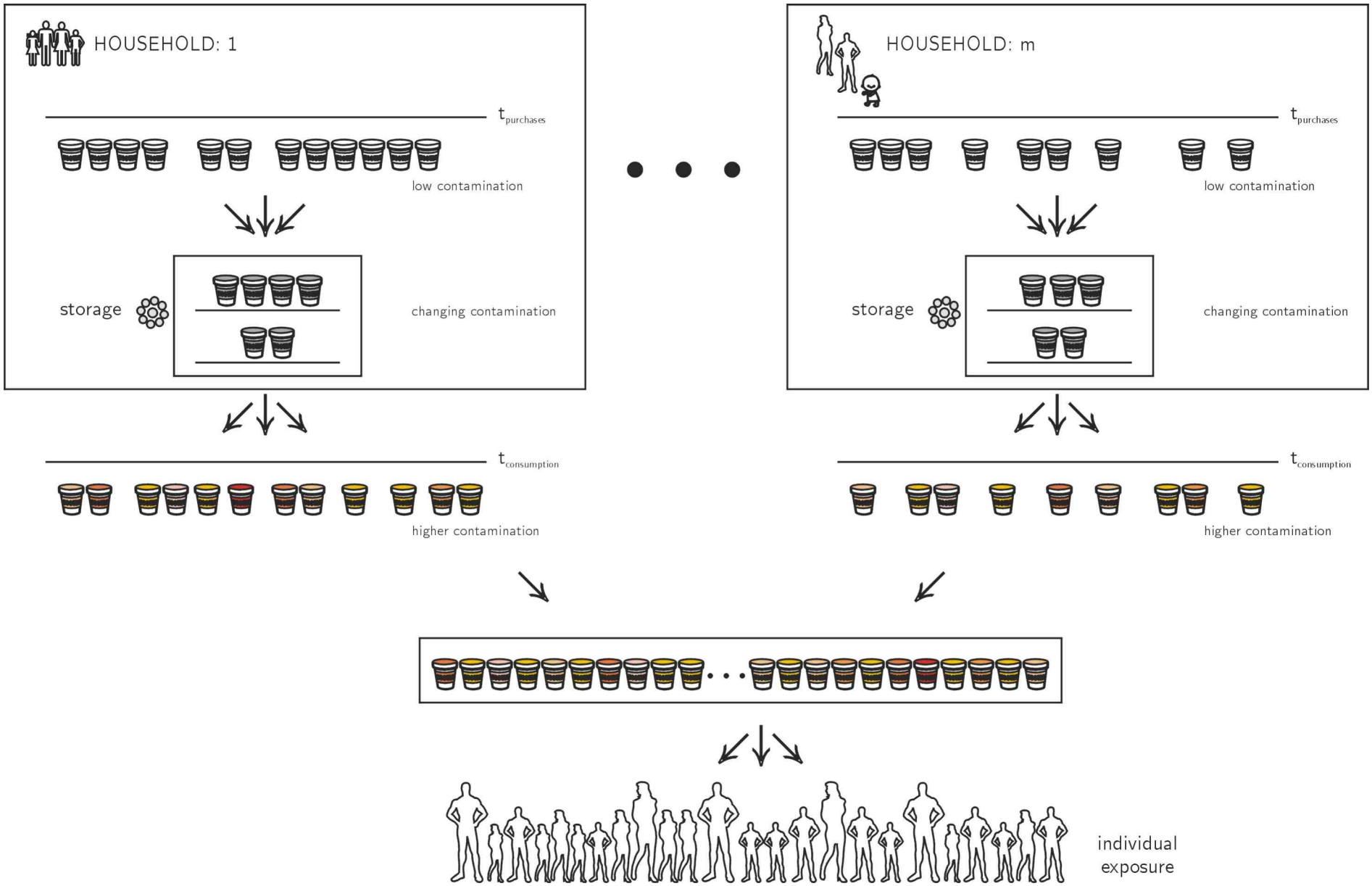
**EVALUATION DE L'EXPOSITION DU CONSOMMATEUR** A PARTIR DE DONNEES DE CONTAMINATION SIMULEES (MULTISOURCES, PRATIQUES DES MENAGES)
Niveau de difficulté: faible à moyen

**PREDIRE LES COEFFICIENTS DE DIFFUSION** DES ADDITIFS DANS LES MATRICES PLASTIQUES PAR SIMULATION DE LA DYNAMIQUE MOLECULAIRE
Niveau de difficulté: moyen à élevé

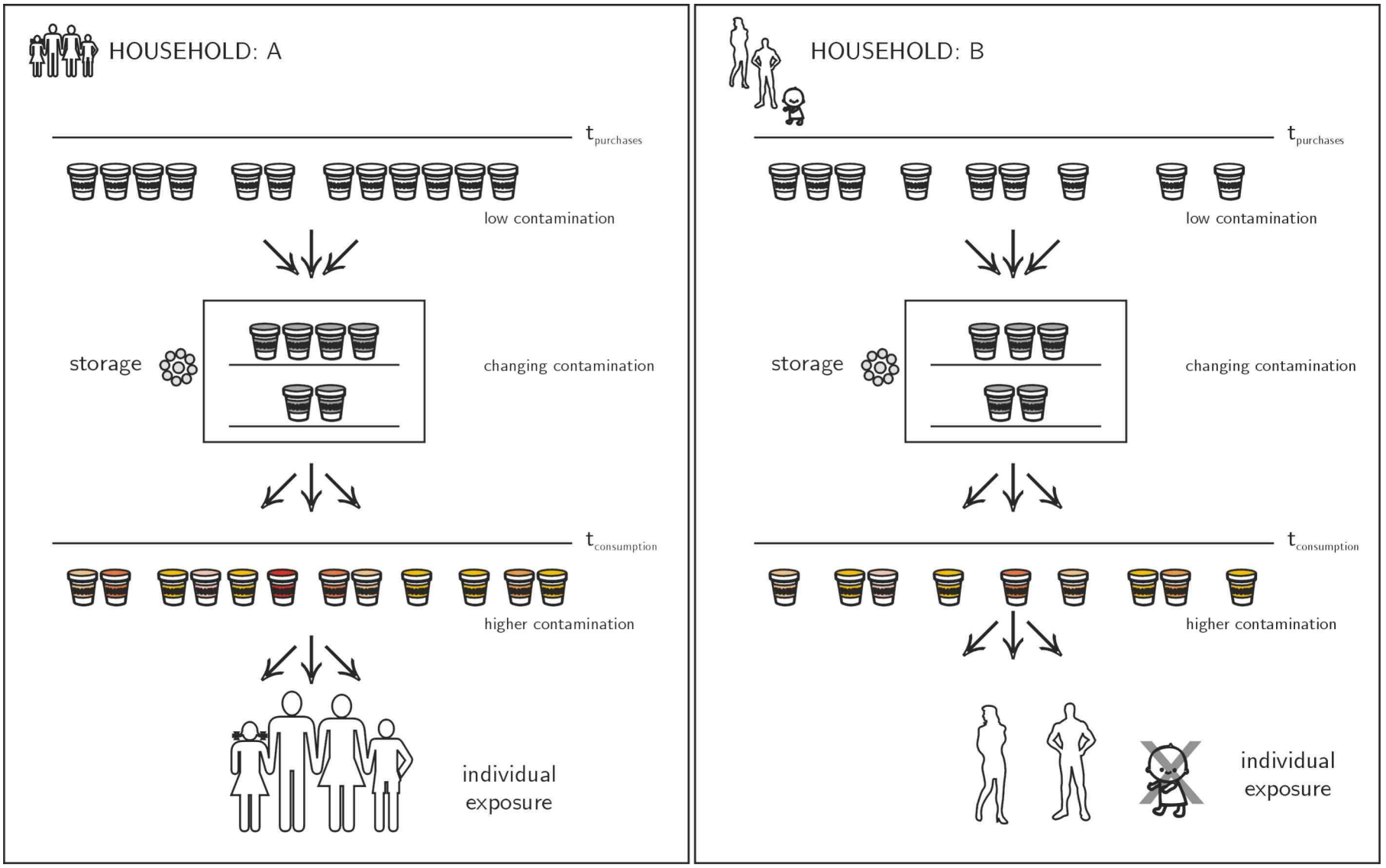
# EVALUATION DE L'EXPOSITION DU CONSOMMATEUR A PARTIR DE DONNEES DE CONTAMINATION SIMULEES

# CONVENTIONAL DESCRIPTION

## CONTAMINATION AND CONSUMPTION ARE INDEPENDENT



# OBJECTIVES: DETAILED RISK ANALYSIS



# OBJECTIVES: DETAILED RISK ANALYSIS

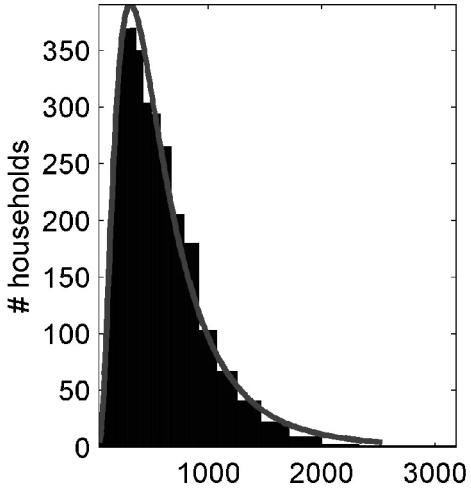
$$E_{k^{th}\ individual} = \frac{1}{365} \cdot \sum_{i=1}^{\overbrace{N_k}^{\text{yearly consumption}}} \underbrace{M_0|_i}_{\text{food weight}} \cdot \underbrace{C_F|_i^{\left(Fo|_i, Bi, K, L\right)}}_{\text{contamination}}$$

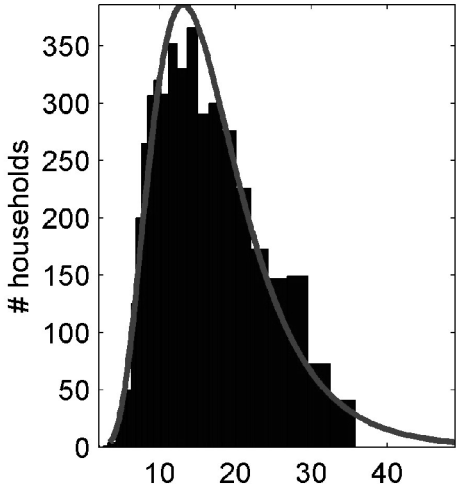
$\mathrm{kg \cdot day^{-1} \cdot person^{-1}}$

$$\underset{household\ /\ individual\ scale}{p_r\left(E \le y\right)} = f\left(\begin{array}{l} \text{food product } \boldsymbol{s}, \text{packaging material } \boldsymbol{s}, \text{migrant } [\boldsymbol{s}] \\ \text{storage cond } \boldsymbol{s}., \text{uncertainty} \\ \text{consumption scenario } \boldsymbol{s} \end{array}\right)$$

# INPUT DATA

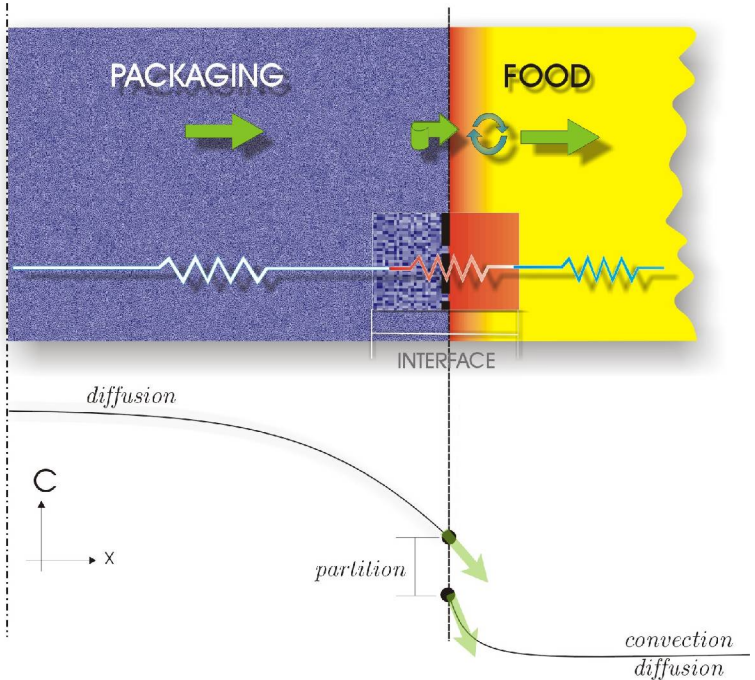
## PURCHASE DATA
(ex. yogurts)



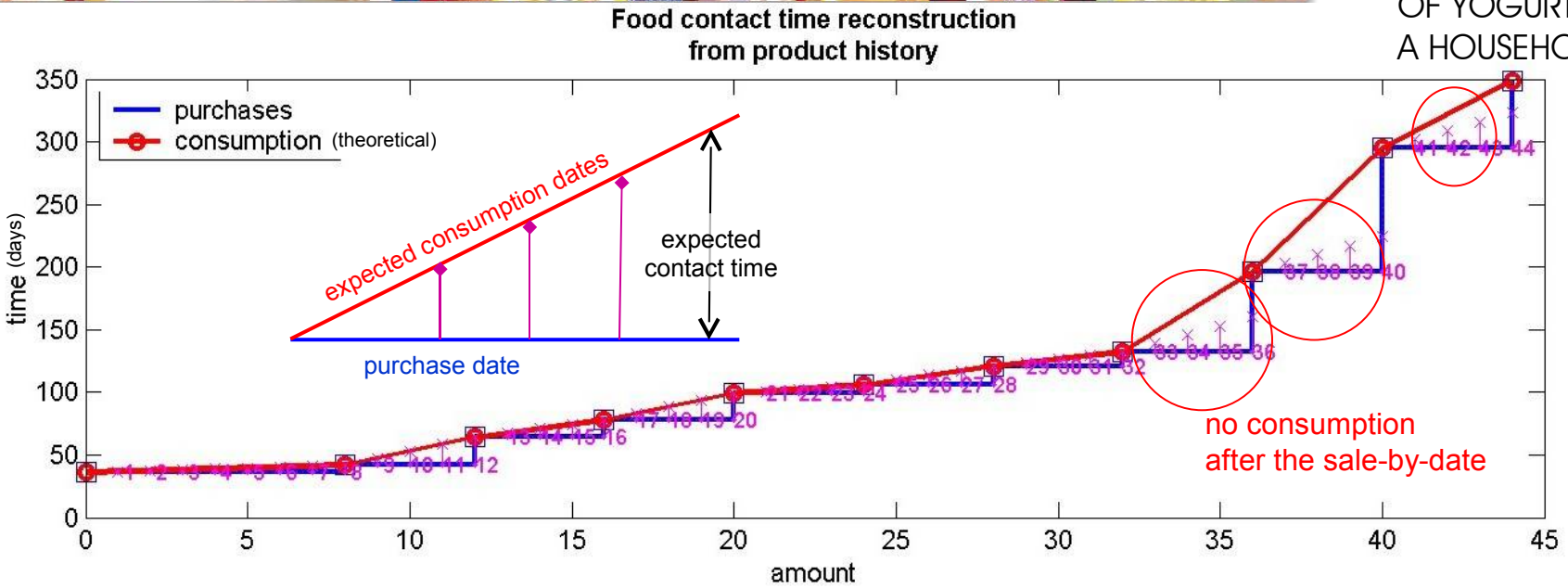

## OUR KNOWLEDGE
(physico-chemistry
Scenarios)

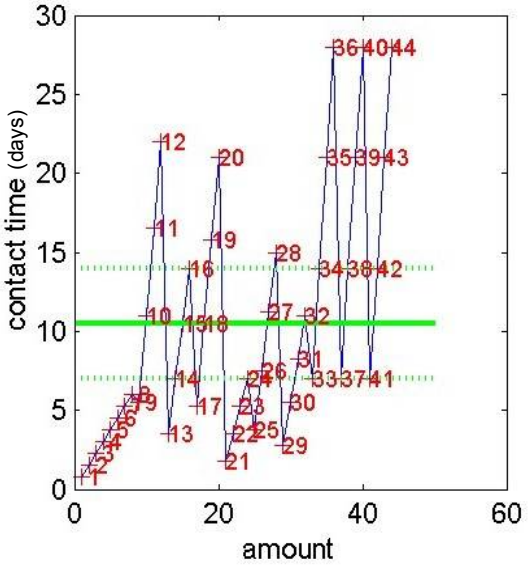
$$p_r\left(C_F \le x\right) = f\begin{pmatrix}\text{food, packaging, migrant}\textit{[s]}\\ \text{storage cond., uncertainty}\end{pmatrix}$$
$$\underset{\textit{product scale}}{}$$

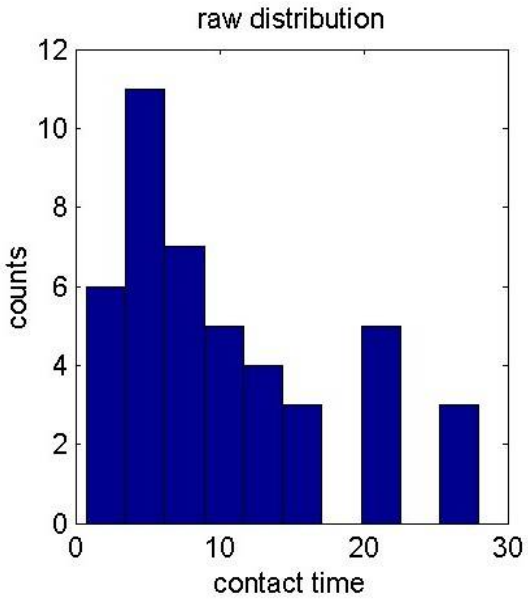


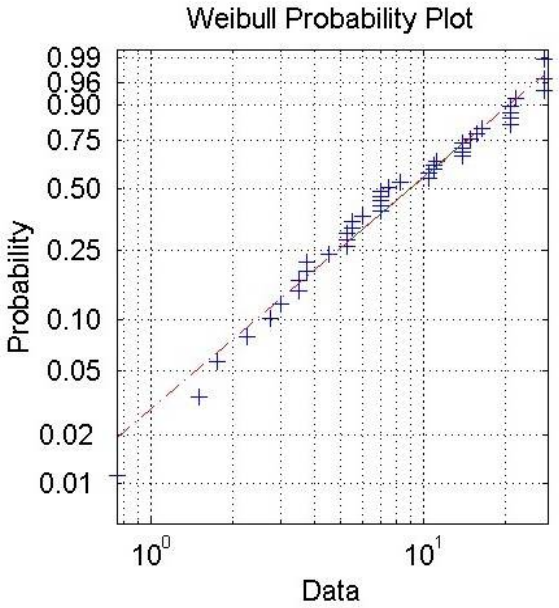
# FROM PURCHASE DATA TO CONTACT TIMES

EXAMPLE:
YEARLY PURCHASE OF YOGURTS OF A HOUSEHOLD

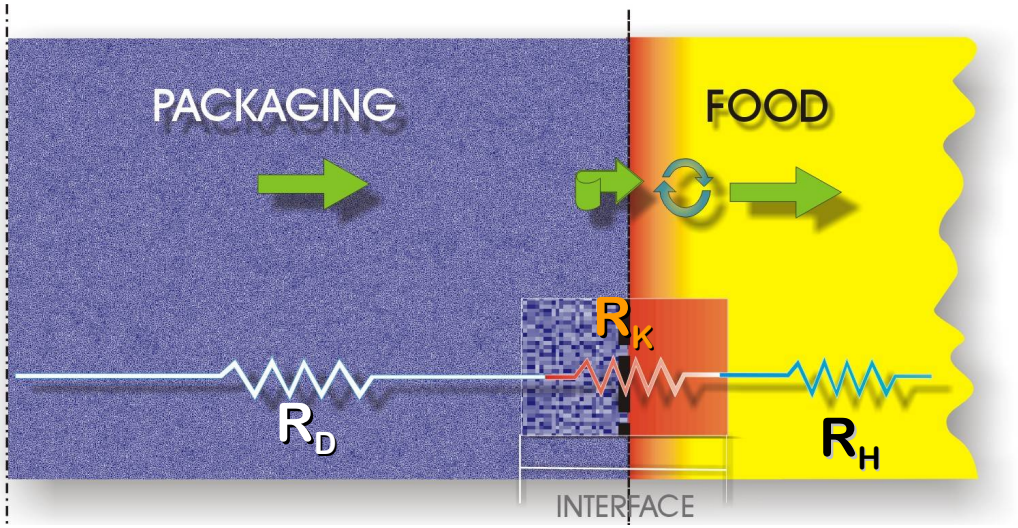


# FROM CONTACT TIMES TO THE CONTAMINATION PREDICTION




| | |
|---|---|
| $0 \le u \le 1$ | Brownian density [-] |
| $Fo = \frac{t \cdot D}{l^2}$ | dimensionless time [-] |
| $x^* = \frac{x}{l}$ | dimensionless position [-] |
| $L = \frac{V_{pack}}{V_{food}} \frac{\rho_{pack}}{\rho_{food}}$ | dilution coefficient [-] |
| $K = \frac{v_{(1)}}{u_{(1)}}$ | partition coefficient [-] |
| $Bi = \frac{R_D}{R_H} = \frac{h \cdot l}{D}$ | Biot number [-] |
| $h$ | mass transfer coefficient [m·s$^{-1}$] |
| $D$ | diffusion coefficient [m$^2$·s$^{-1}$] |
| $t$ | contact time [s] |
| $l$ | thickness of the layer in contact [m] |
| $c_0$ | initial concentration in packaging [kg·kg$^{-1}$] |

*Transport equation* $\frac{\partial u}{\partial Fo} = \frac{\partial u}{\partial x^*} \quad 0 \le x^* \le 1$

*BC & IC*
$$\begin{cases} j^* = -\left.\frac{\partial u}{\partial x^*}\right|_{x^*=1} = Bi \cdot K \cdot \left( u_{|x^*=1} - \frac{\overline{v}^*}{K} \right) \; ; \; \left.\frac{\partial u}{\partial x^*}\right|_{x^*=0} = 0 \\ u_{(x,Fo=0)} = 1 \end{cases}$$

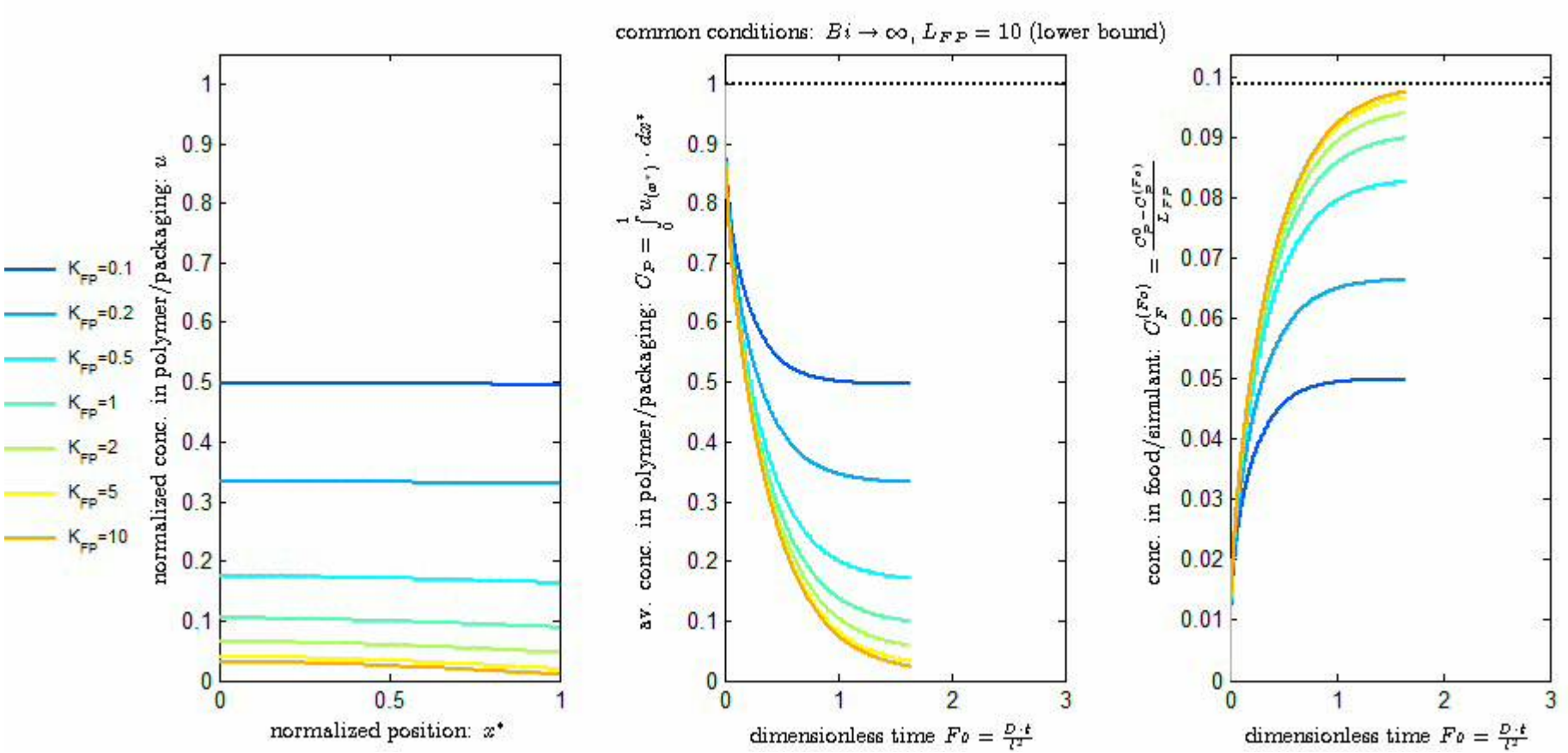
*Migrant balance*
$$\begin{cases} \overline{u} + \frac{\overline{v}_\infty}{L} \cdot \overline{v}^* = 1 \\ \overline{v}_\infty = \left( \frac{1}{K} + \frac{1}{L} \right)^{-1} \end{cases}$$

*Concentration in food: $c_F$*

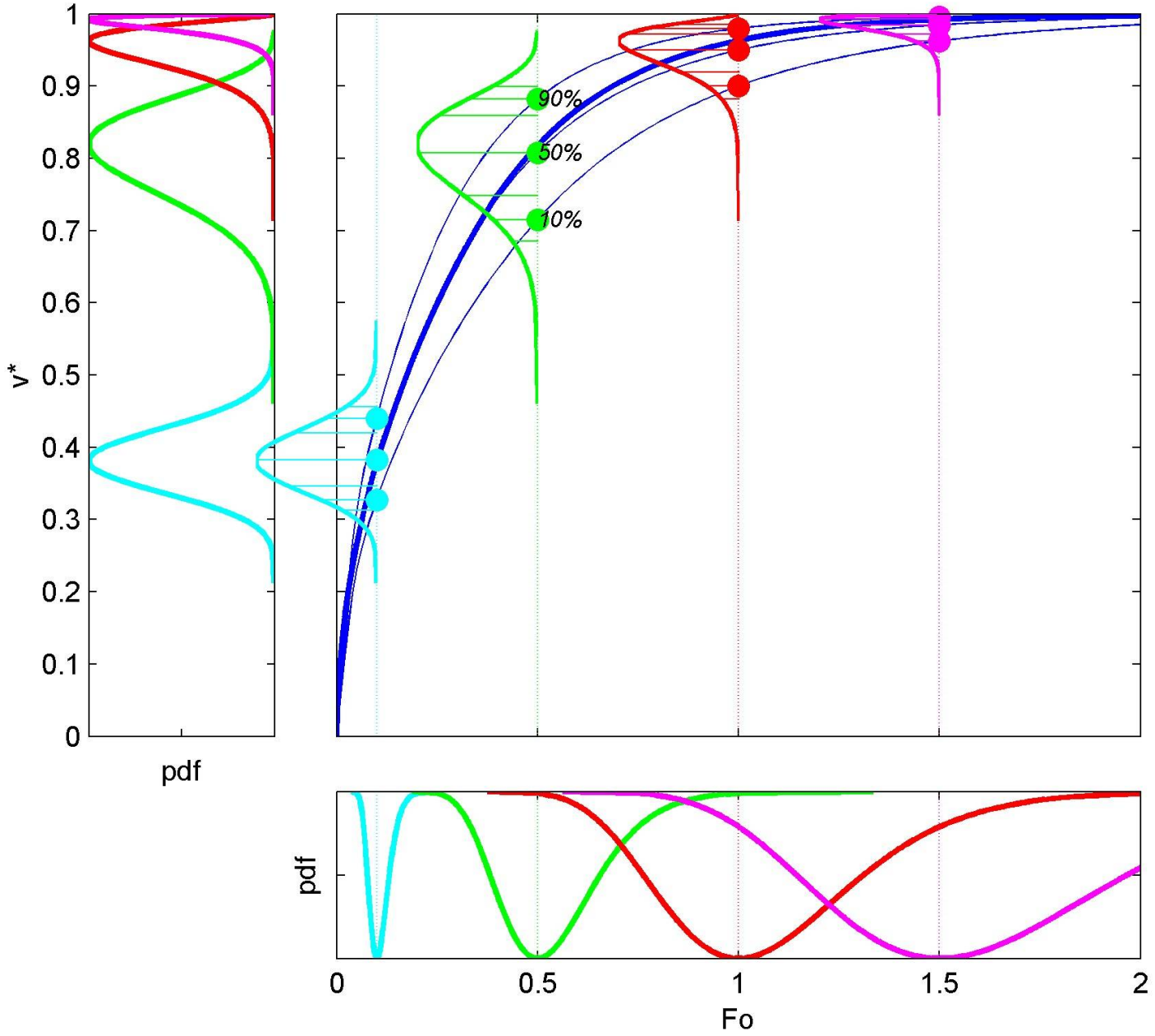
$$c_F(Fo,Bi,K,L) = c_0 \cdot \overline{v}_\infty(K,L) \cdot \overline{v}^*(Fo,Bi,K,L)$$

sensitivity: + ++ +++

# FROM CONTACT TIMES TO THE CONTAMINATION PREDICTION




See the video: http://h29.univ-reims.fr/virtual/simKeffect.avi
(more similar videos available at: http://h29.univ-reims.fr in the "virtual experiments" section:)


1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
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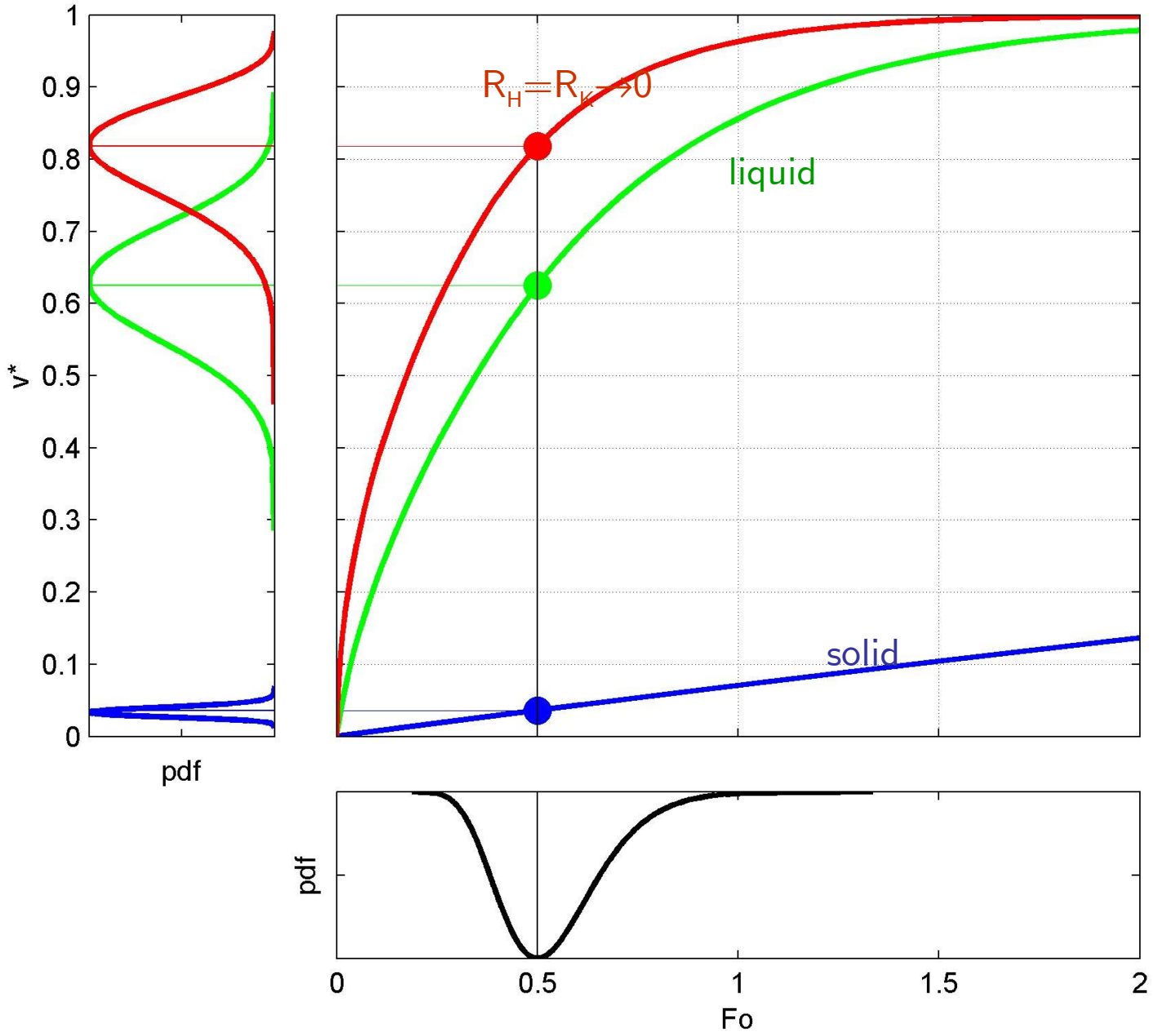
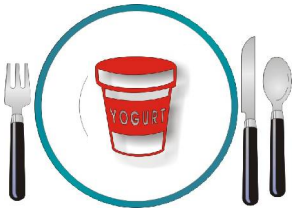


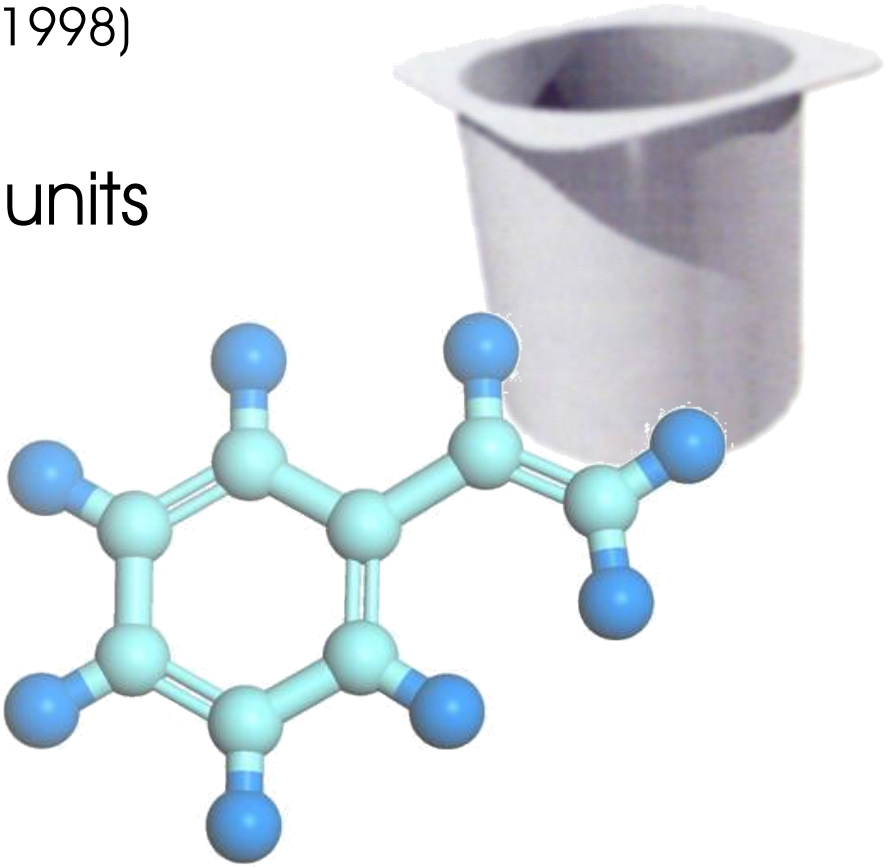

$Fo^*(s_D = 0.2)$

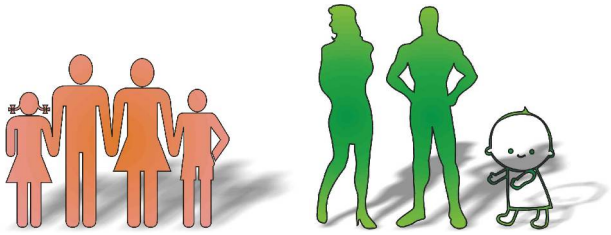
$D^* \sim \log_{10} N(0, s_D)$

# EXAMPLE: EXPOSURE TO STYRENE FROM YOGURTS PACKED IN PS




6122 Households (year 1998)
221,190 Purchases
1,930,257 Purchased units





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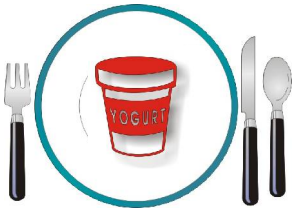
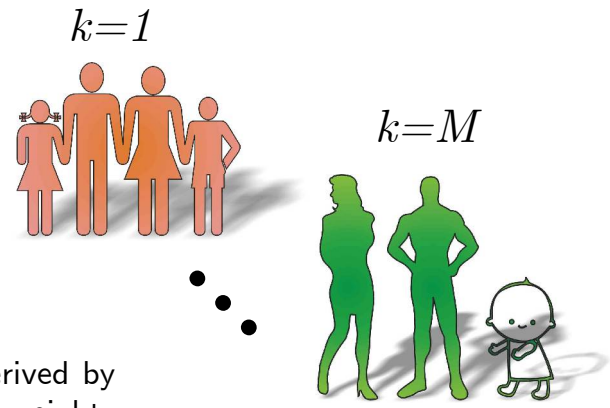



For an household $k$, of size $P_k$, the exposure of the "typical" consumer, $E_k$, that consumes $N_k$ yoghurts in pots of weight $M_0$ (typically 0.125 kg), is efficiently calculated by factorizing $E_k$ as a sum of $N_k$ independent variables:

$$E_k = \frac{c_0 \cdot \overline{v}_\infty^*}{365 \cdot P_k} \cdot \sum_{i=1}^{N_k} \overline{v}_i^* \left( Fo_i, Bi, K, L \right)$$




Exposure of a population of M=4,671 households (14,649 persons) is finally derived by combining the independent distributions of $\{E_k\}_{k=1...4671}$ respectively to the weights $\{P_k\}_{i=1..4671}$.

$$pdf\left[\sum_{i=1}^{N_k} \overline{v}_i^*\right] ?$$

$$V_\Sigma^{(N_k)} = V_1 \otimes \cdots \otimes V_i * \cdots \otimes V_{N_k} =$$

$$= V_\Sigma^{(P_1^n)} \otimes V_\Sigma^{(P_1^n)} = \underbrace{V_\Sigma^{(P_1^{n-1})} \otimes V_\Sigma^{(P_2^{n-1})}}_{V_\Sigma^{(P_1^n)}} \otimes \underbrace{V_\Sigma^{(P_3^{n-1})} \otimes V_\Sigma^{(P_4^{n-1})}}_{V_\Sigma^{(P_2^n)}}$$

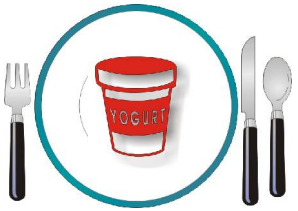
$$= \underbrace{V_\Sigma^{(P_1^{n-2})} \otimes V_\Sigma^{(P_2^{n-2})}}_{V_\Sigma^{(P_1^{n-1})}} \otimes \underbrace{V_\Sigma^{(P_3^{n-2})} \otimes V_\Sigma^{(P_4^{n-2})}}_{V_\Sigma^{(P_2^{n-1})}} \otimes \underbrace{V_\Sigma^{(P_5^{n-2})} \otimes V_\Sigma^{(Q_6^{n-2})}}_{V_\Sigma^{(P_3^{n-1})}} \otimes \underbrace{V_\Sigma^{(P_7^{n-2})} \otimes V_\Sigma^{(P_8^{n-2})}}_{V_\Sigma^{(P_4^{n-1})}}$$

$$= \cdots$$

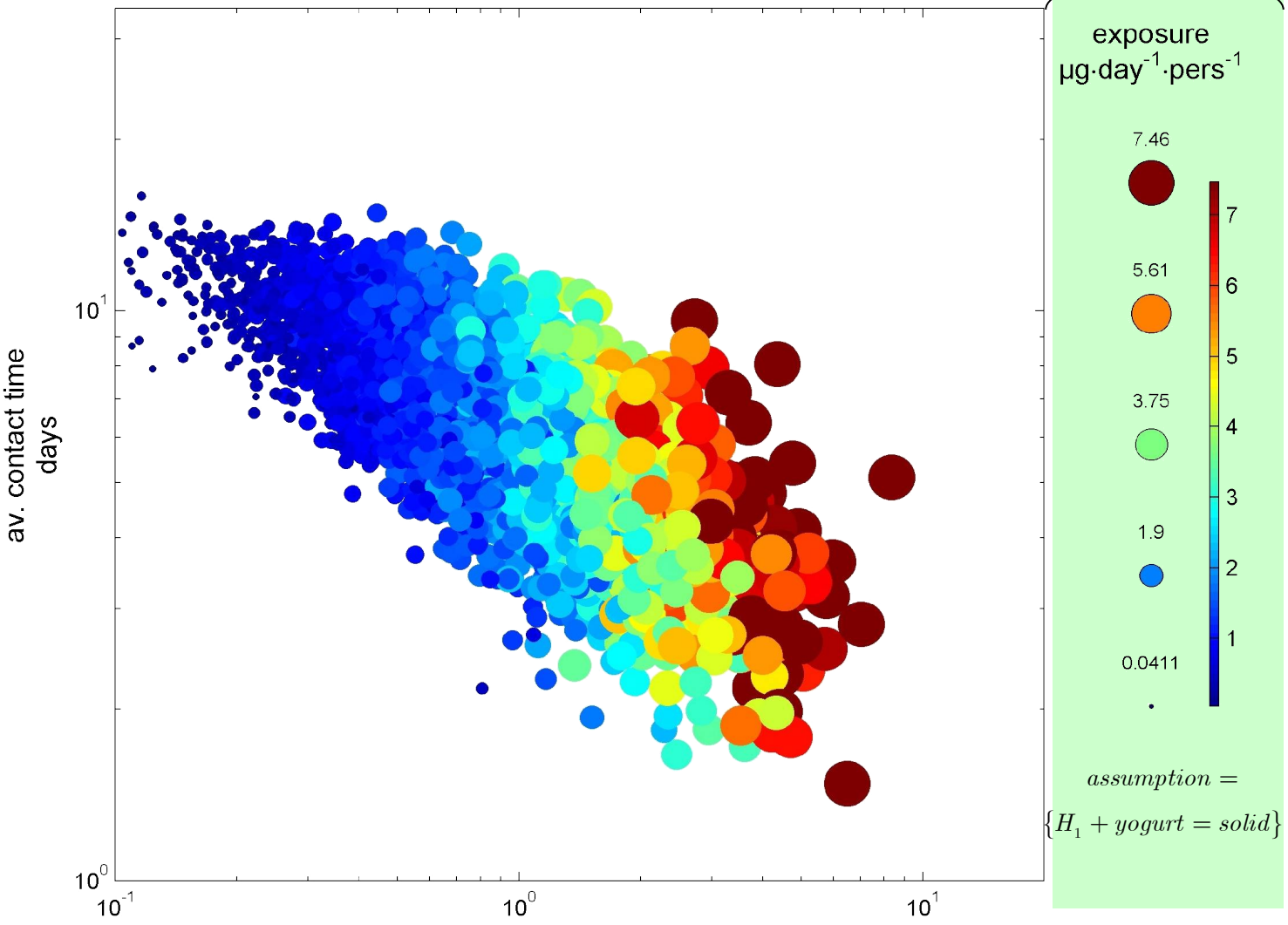
$$V_i = pdf\left[\left\{\overline{v}_i^*\right\}_{i=1...N_k}\right]$$

$$\bigcup_{j=1}^{N_k} P_j^1 = 1 \ldots N_k$$

# EXAMPLE: EXPOSURE TO STYRENE FROM YOGURTS PACKED IN PS




95th percentile




exposure
µg·day$^{-1}$·pers$^{-1}$

7.46

5.61

3.75

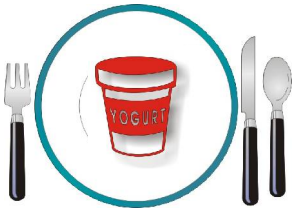
1.9

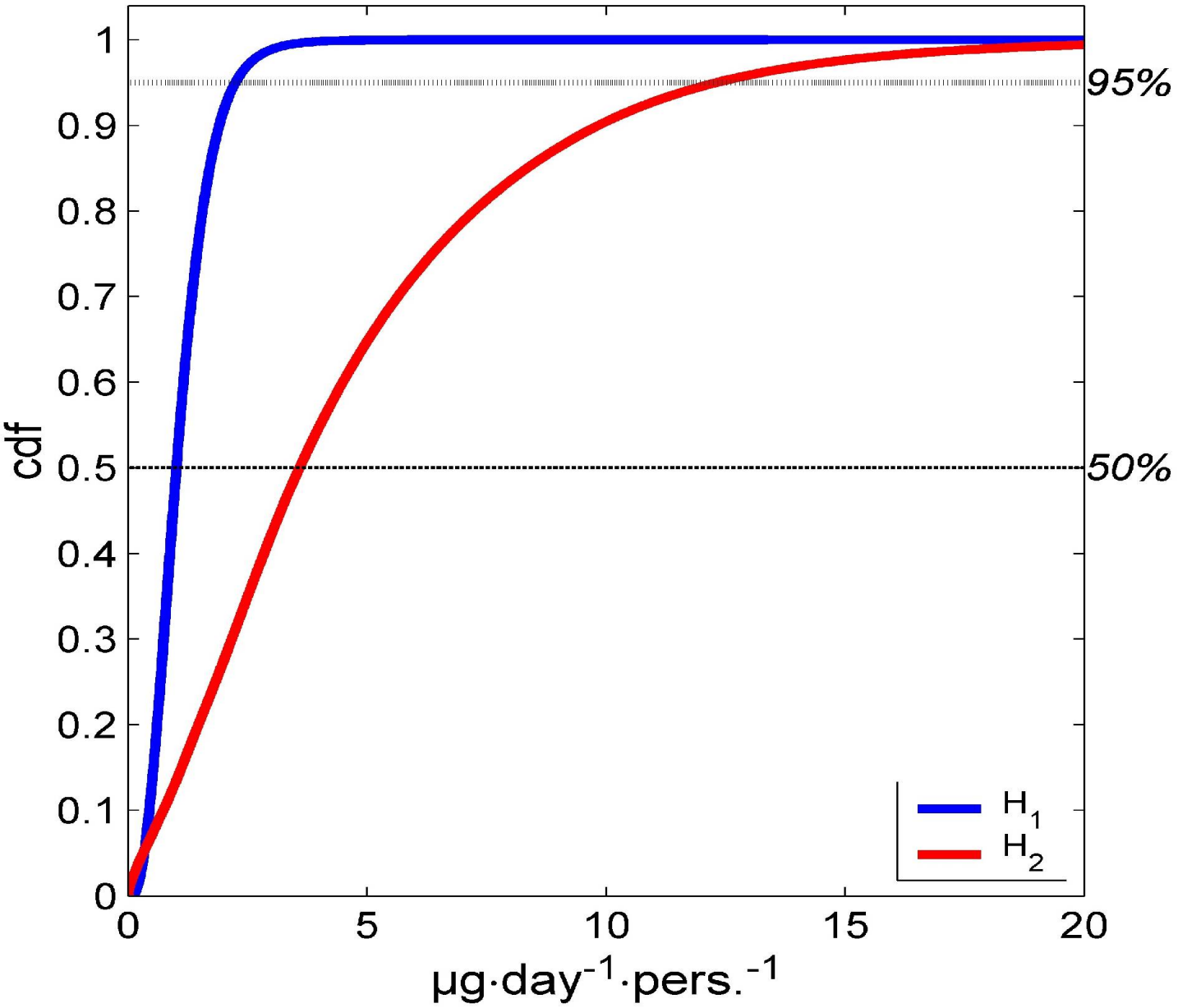
0.0411

7
6
5
4
3
2
1

$assumption =$
$\{H_1 + yogurt = solid\}$

# EXAMPLE: EXPOSURE TO STYRENE FROM YOGURTS PACKED IN PS



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Toxicology 144 (2000) 39–50

TOXICOLOGY

www.elsevier.com/locate/toxicol

# Estimation of human exposure to styrene and ethylbenzene

Weici Tang, Ingrid Hemm, Gerhard Eisenbrand *

*Department of Chemistry, Division of Food Chemistry and Environmental Toxicology, University of Kaiserslautern, Erwin-Schroedinger-Str., D-67663 Kaiserslautern, Germany*

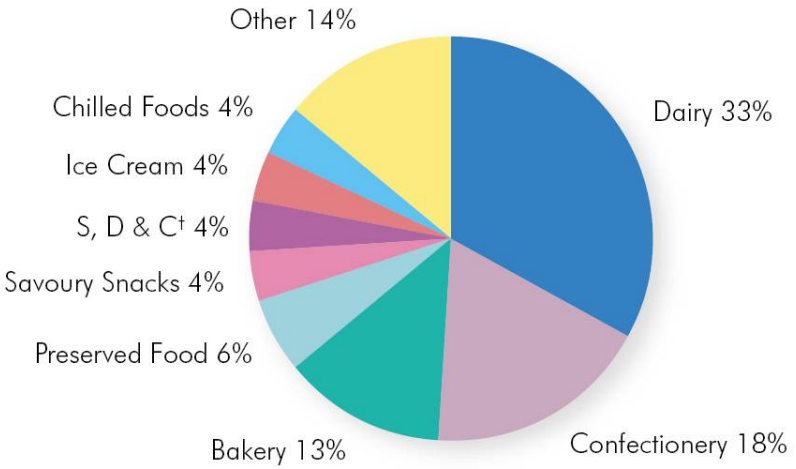
Dedicated to Professor Dr K.J. Netter

**Abstract**

In the present studies, human exposure to styrene and to ethylbenzene (EB) is assessed on the basis of literature data. Total styrene and total EB exposure result from inhalation and from food intake. Styrene and EB inhaled represent the greatest proportion of the total intake. Styrene and EB content in food is mainly caused by migration from polymer packaging material. The daily styrene exposure is estimated to range from 18.2 to 55.2 μg/person, corresponding to an annual exposure of 6.7 to 20.2 mg/person. The daily EB exposure is estimated to be about 130 μg/person, corresponding to an annual exposure of 46 mg/person. Cigarette smoking is another important factor for styrene and EB intake by smokers. 

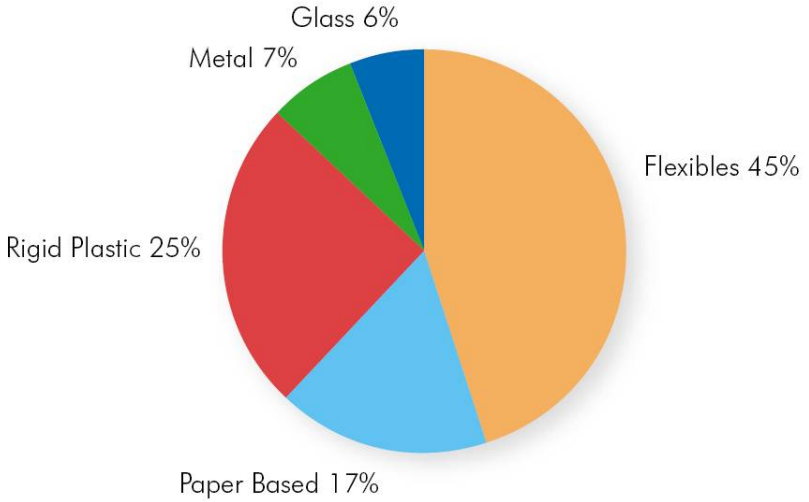
*Keywords:* Styrene; Ethylbenzene; Human exposure

# EXTENSIONS


>4000 Food Types
>200 Packaging types
>300 Contaminants
Variable industrial practices
Variable household practices

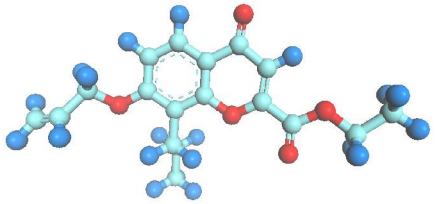
ONLINE SOFTWARES AND DATABASES (EU VALIDATED)



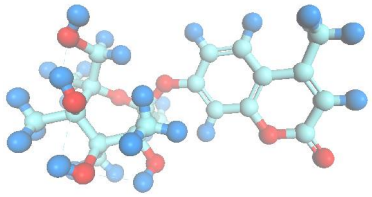
# PREDIRE LES COEFFICIENTS DE DIFFUSION DES ADDITIFS DANS LES MATRICES PLASTIQUES PAR SIMULATION DE LA DYNAMIQUE MOLECULAIRE

Question de recherche très générale
(incluse au programme de recherche 2006-2010
sur le vieillissement des matrériaux composites industriels
Participants: CNRS-CEA-INRA-EDF-Laborelec-Nexans)

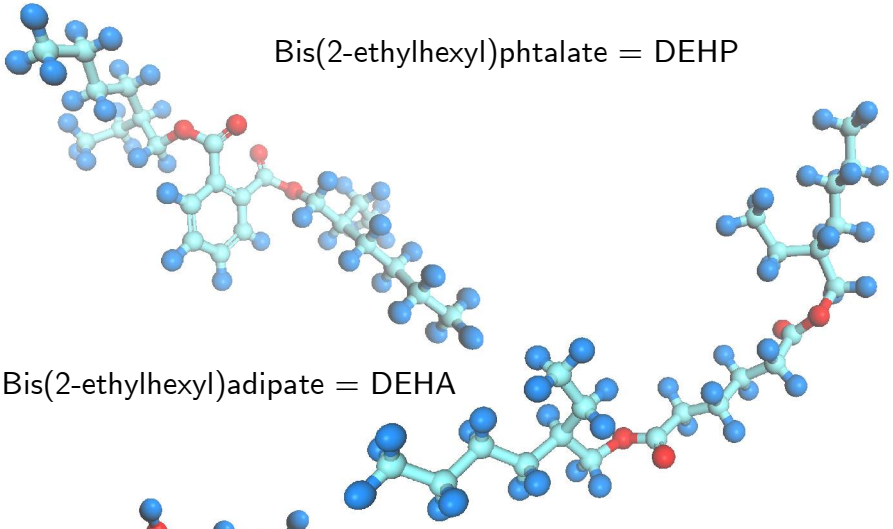
# TYPICAL CONTAMINANTS



PCC
(Benzopyran-carboxylic-acid_oxo-propenyloxy-propyl_ethylester)

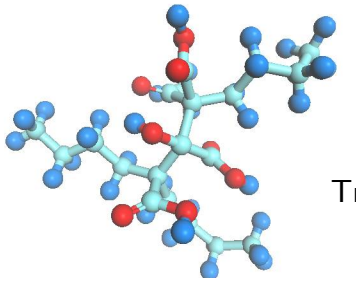


4-Methylumbelliferyl-beta-D-galactopyranoside

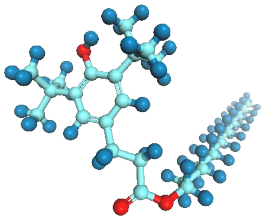


Bis(2-ethylhexyl)phtalate = DEHP

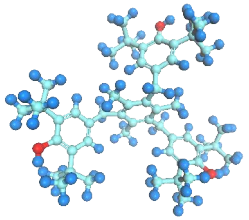
Bis(2-ethylhexyl)adipate = DEHA



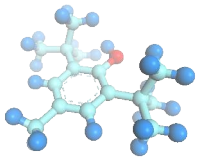
Tributyl-acetyl citrate



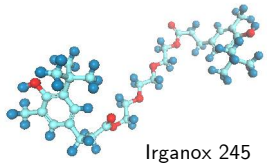
Irganox 1076



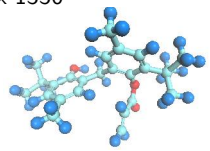
Irganox 1330



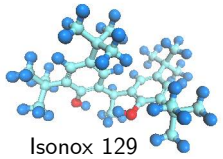
BHT



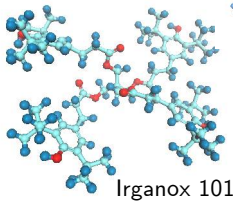
Irganox 245



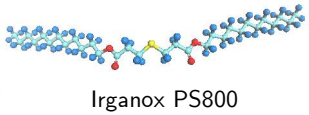
Irganox 3052



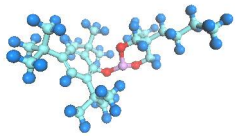
Isonox 129



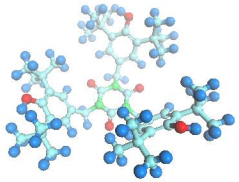
Irganox 1010



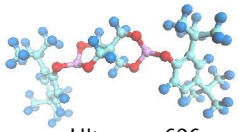
Irganox PS800



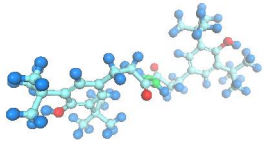
Ultranox 640



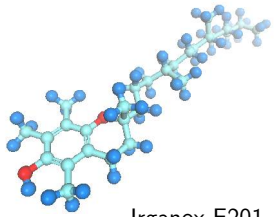
Irganox 3114



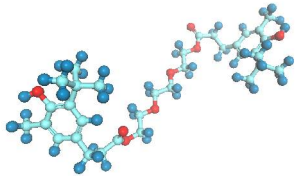
Ultranox 626

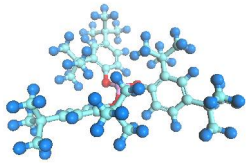


Irganox MD1024

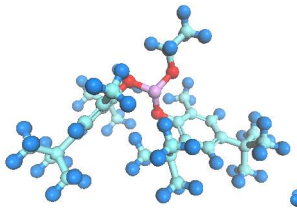


Irganox E201

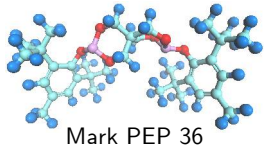




Irgafos 168



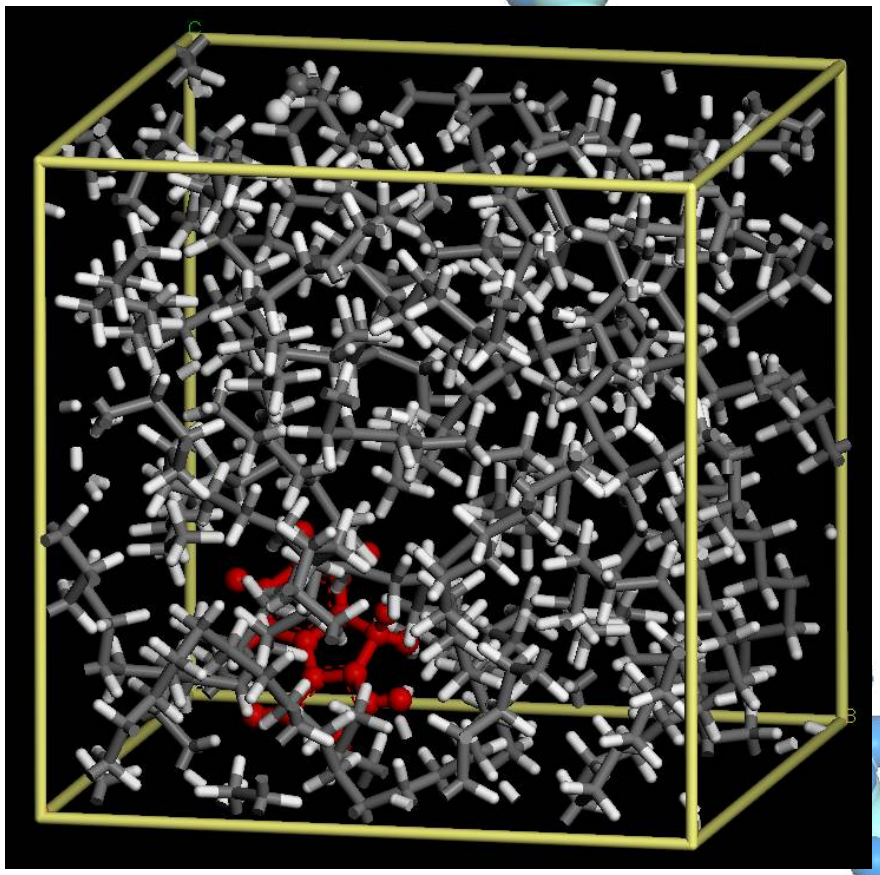
Irgafos 38



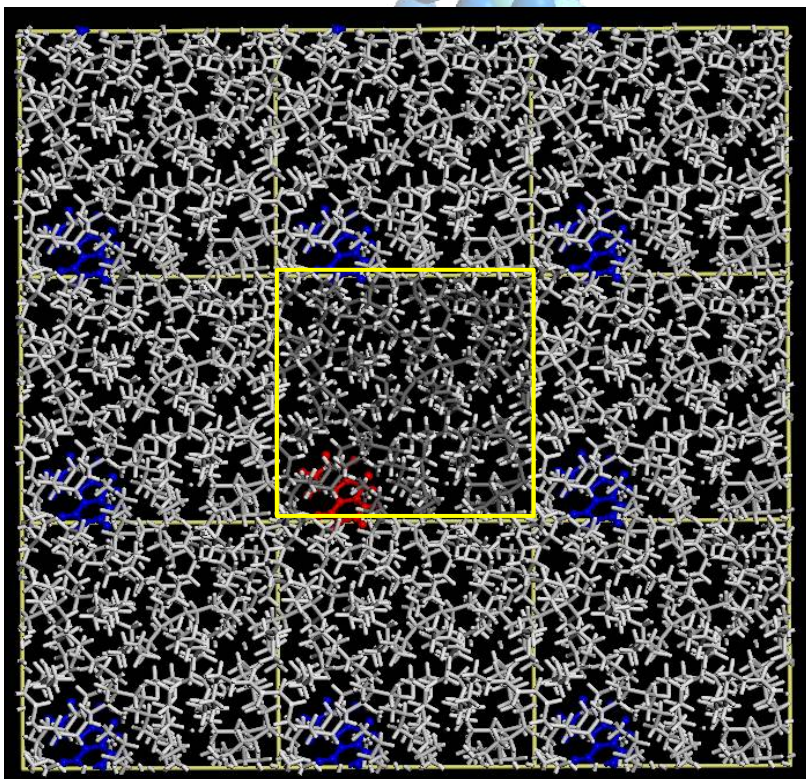
Mark PEP 36

# PRINCIPLES OF MOLECULAR DYNAMICS

CELL = POLYMER + DIFFUSANT

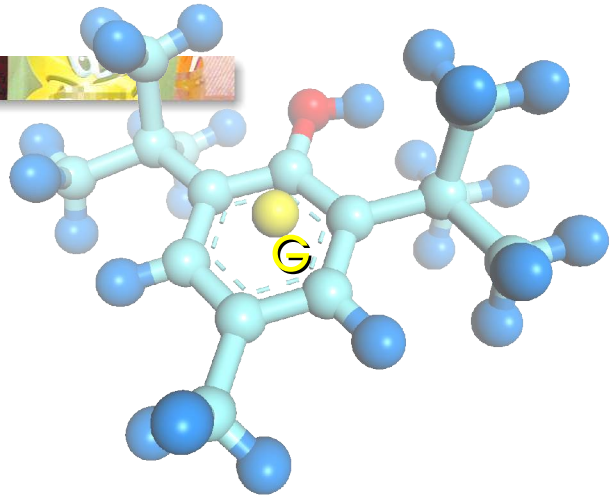


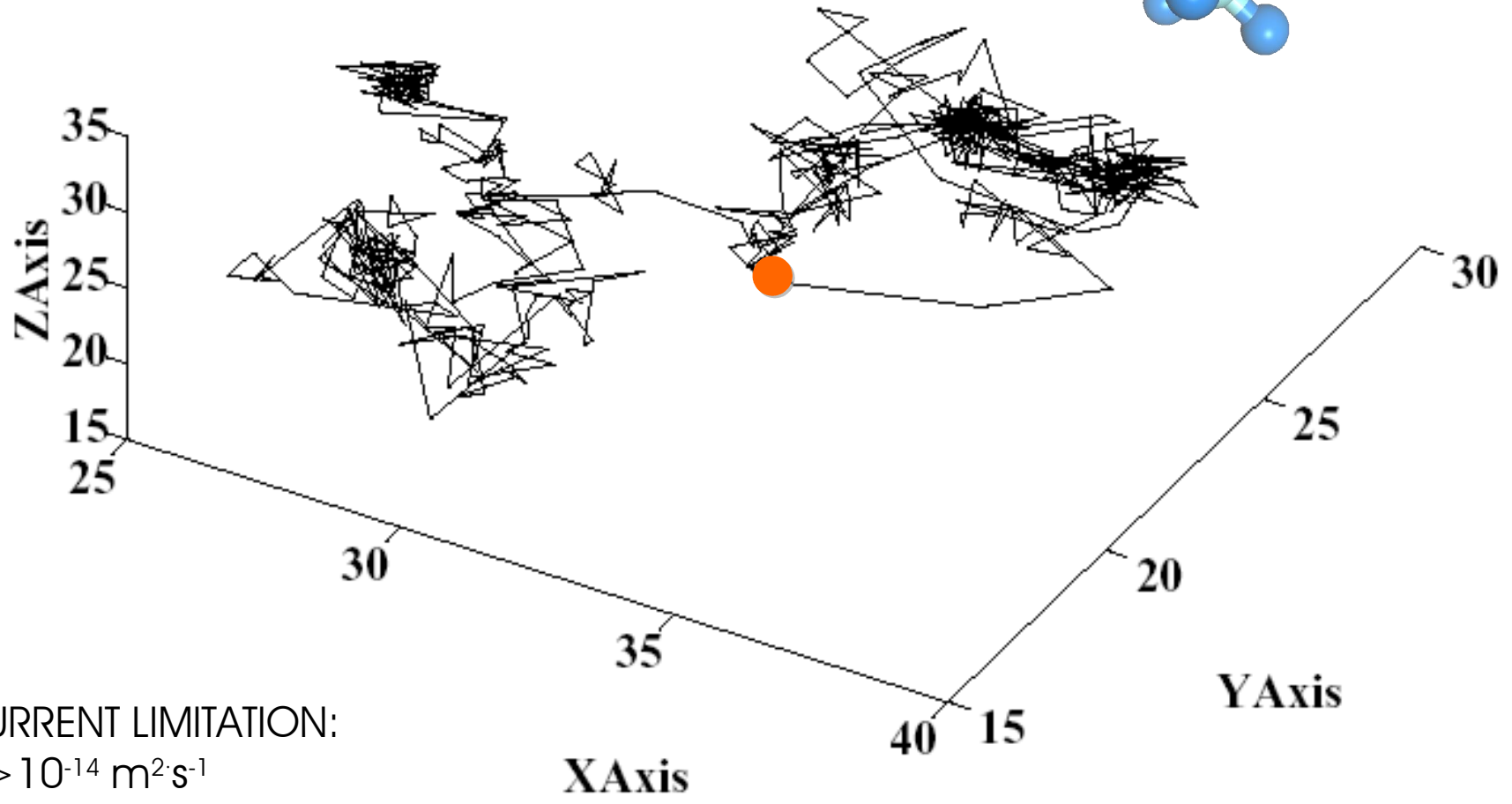
PERIODIC BOUNDARY CONDITIONS



# DERIVATION OF D FROM THE CENTER OF MASS

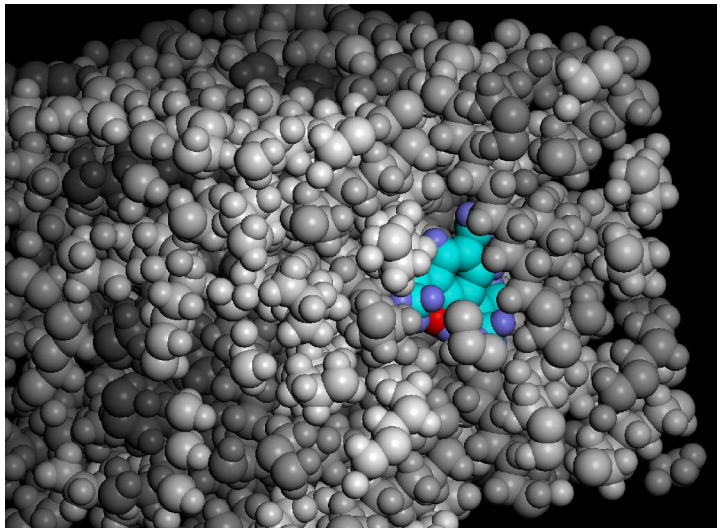
$$D_{Einstein} = \lim_{t \to \infty} \frac{1}{6} \cdot \frac{\partial}{\partial t} \underbrace{\left\langle \left( \vec{x}_G^{(t)} - \vec{x}_G^{(t_0)} \right)^2 \right\rangle}_{msd}$$

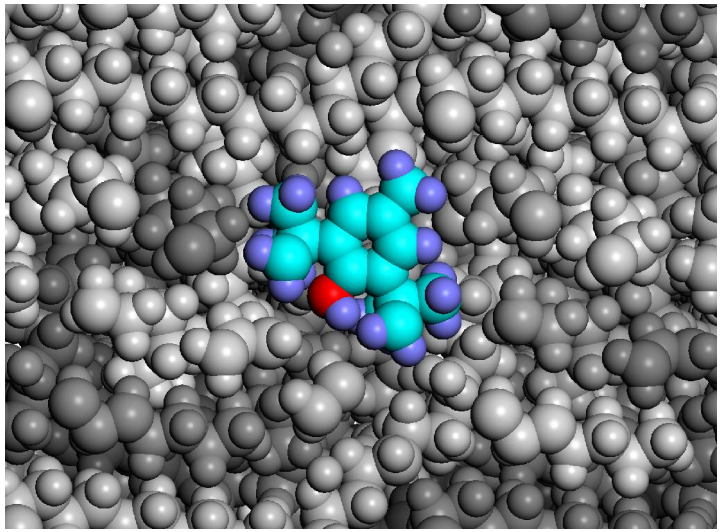


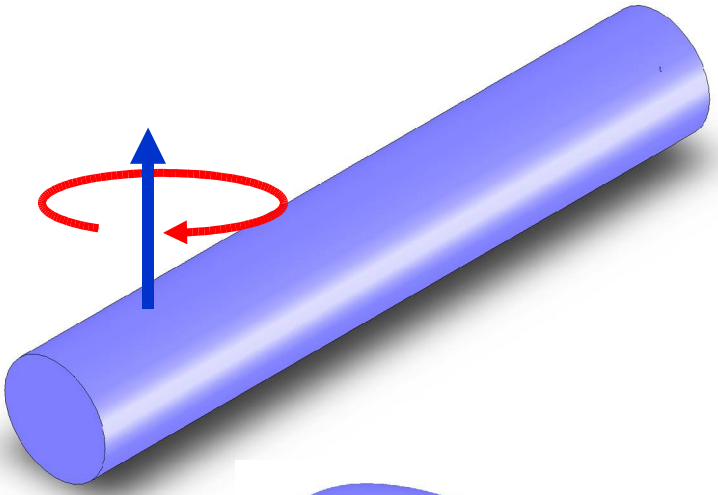

CURRENT LIMITATION:
$D > 10^{-14}\ m^2 \cdot s^{-1}$

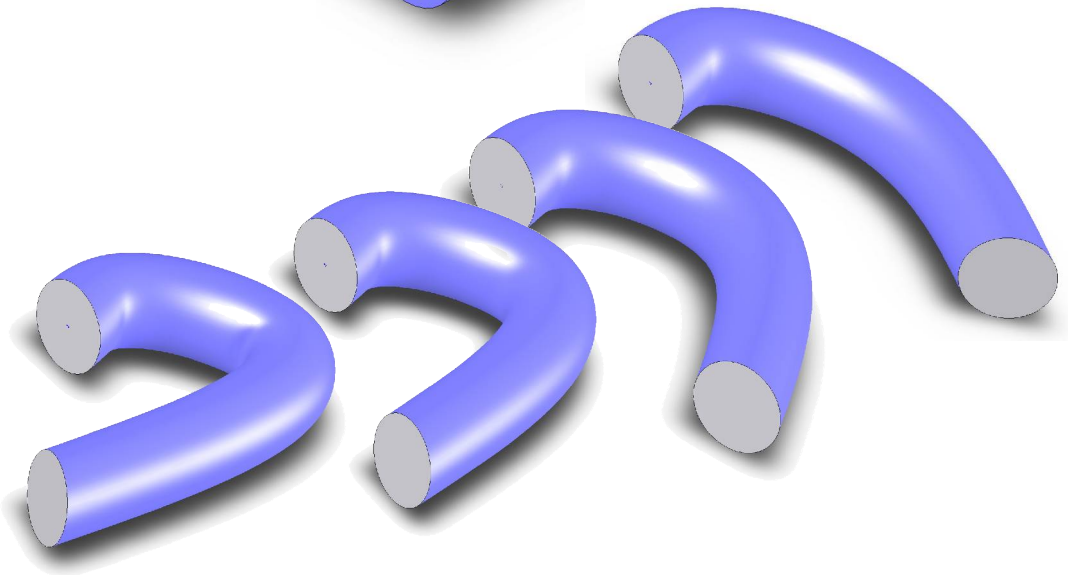
# TRANSLATION MECHANISMS OF MEDIUM-SIZED MOLECULES IN DENSE MEDIA





TRANSLATION
BY REORIENTATION
(RIGID BODY)

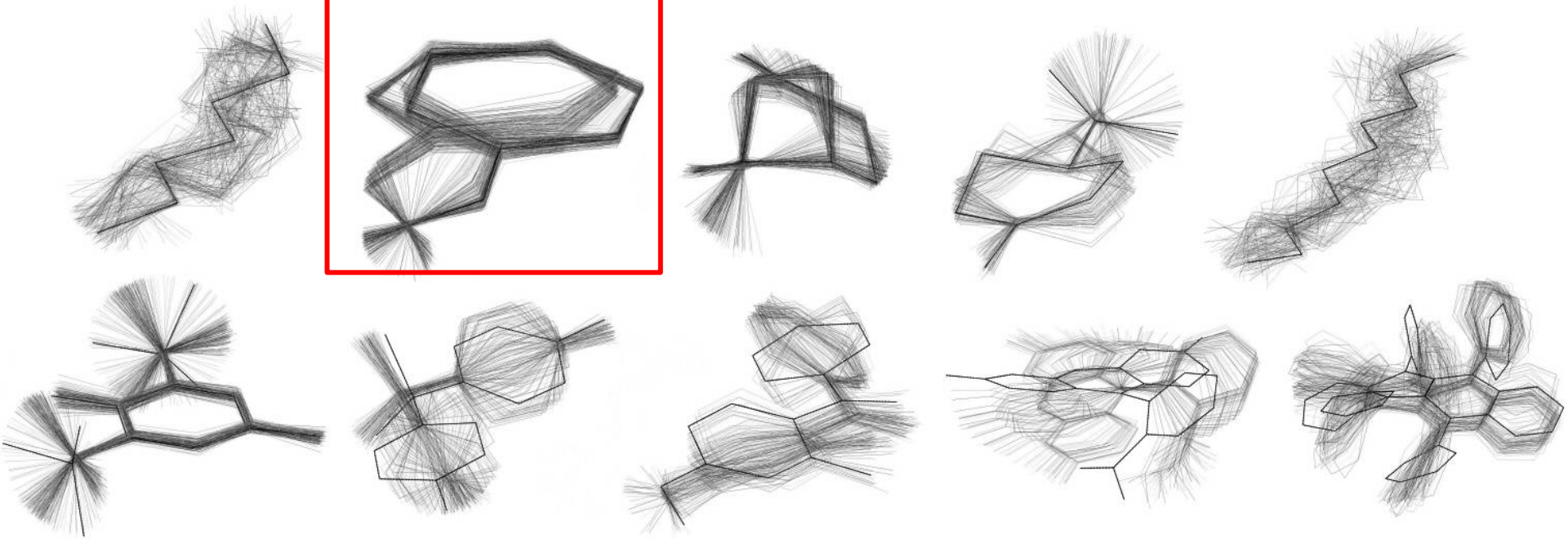




TRANSLATION
BY CONTOUR FLUCTUATION
(DEFORMABLE BODY)

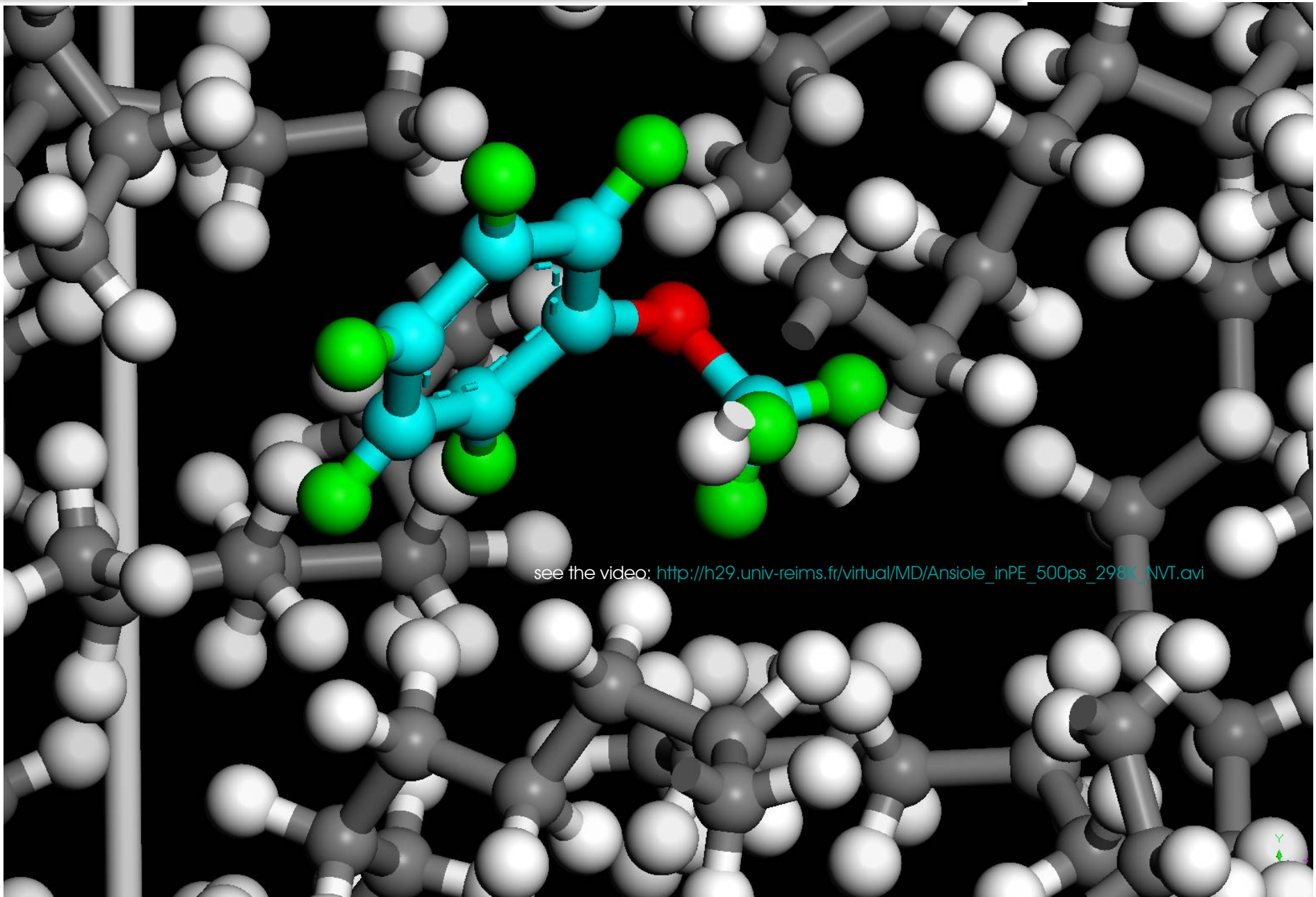
# NON-TRANSLATING FLUCTUATIONS = MICROSTATES

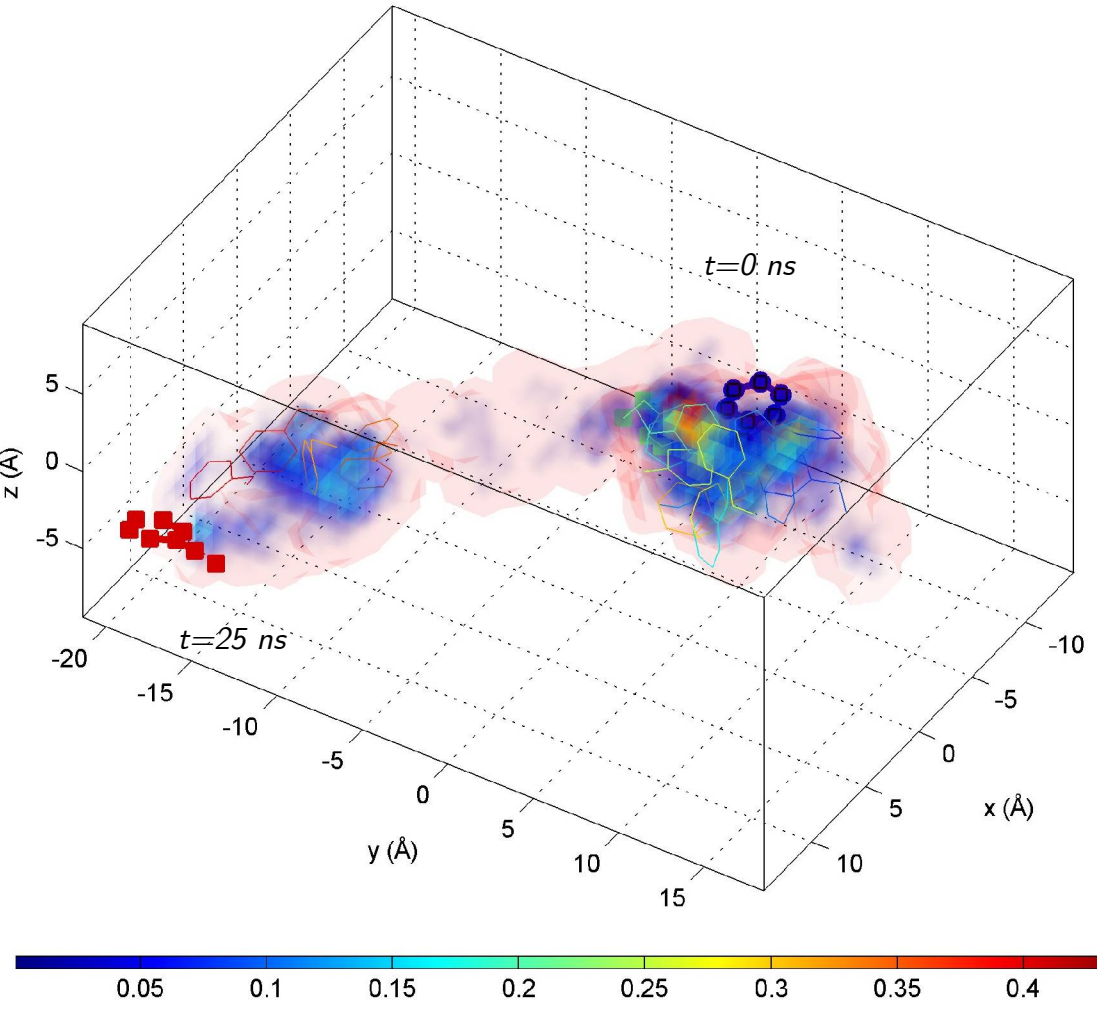
ANISOLE



ALL SAMPLED CONFORMATIONS HAVE THE SAME CENTER OF MASS
(NO TRANSLATION)

# ENTROPIC TRAPPING IN DENSE MEDIA: INFREQUENT TRANSLATIONS









residence time (ps·Å$^{-3}$)


HOW TO DETECT
A HOP (= TRANSLATION)
IN A FRACTAL TRAJECTORY ?


HOW TO PREDICT
CONFINEMENT ?
(distribution of waiting times)

see the videos
http://h29.univ-reims.fr/virtual/MD/anisole16_seq.avi
http://h29.univ-reims.fr/virtual/MD/anisole16_resid_rotation.avi

2a

$$MSD\left(\begin{array}{c}\text{simulation time}\\ \hat{t}\end{array}\;,\;\begin{array}{c}\text{time scale}\\ \overline{\tau}\end{array}\right)=$$

$$\left\langle \left\| \vec{x}_{G,t} - \vec{x}_{G,t-\tau} \right\|^2 \right\rangle_{t-4.5\cdot\tau\le t\le t+5.5\cdot\tau}$$

TOTAL VARIANCE AT THE SCALE τ

V

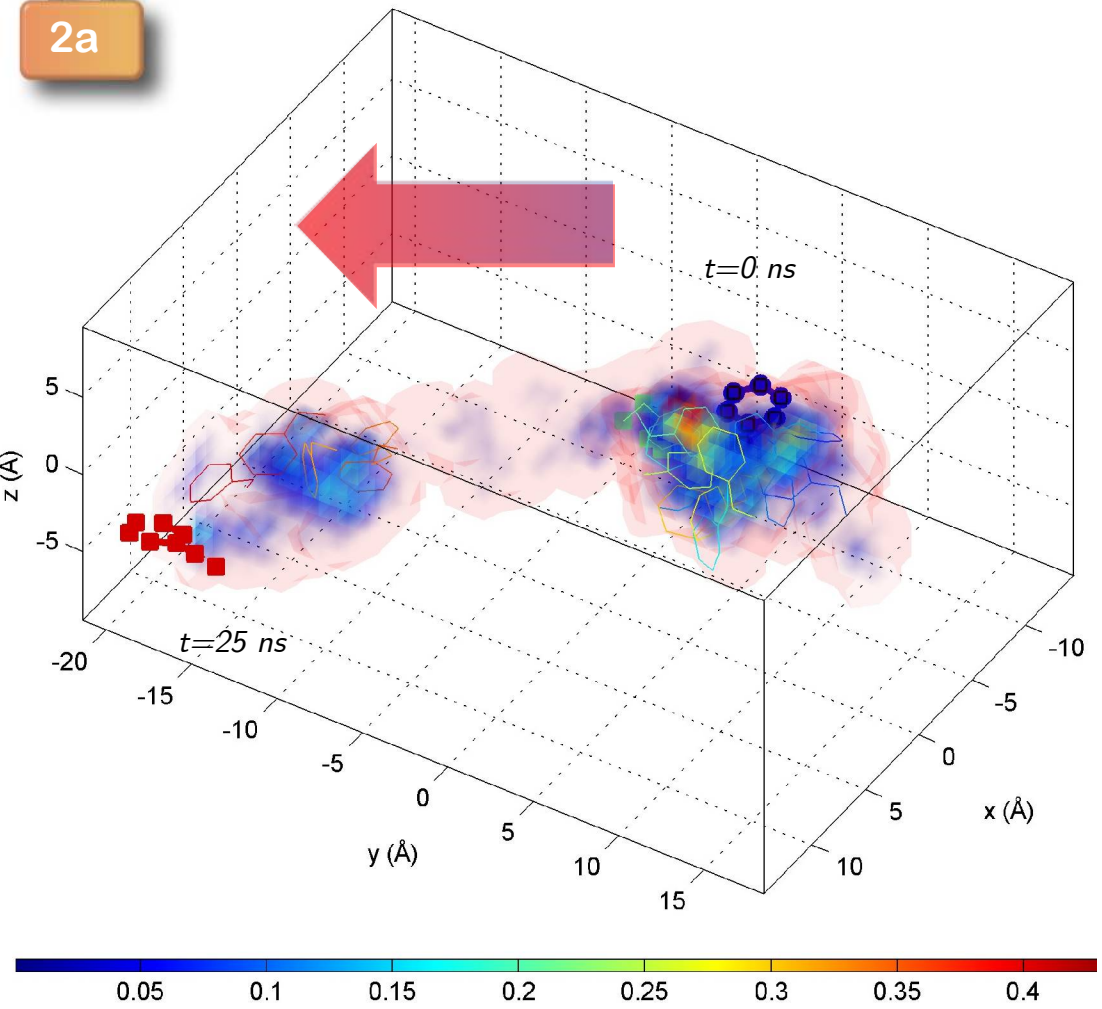
$$MSC\,(t,\tau)=$$

$\vec{x}'_i$ : related to a molecular frame

$$\frac{\left\langle m_i \left\| \left(\vec{x}'_{i,t} - \vec{x}'_{G,t}\right) - \left(\vec{x}'_{i,t-\tau} - \vec{x}'_{G,t-\tau}\right) \right\|^2 \right\rangle_{t-4.5\cdot\tau\le t\le t+5.5\cdot\tau,\,i=1..n}}{\left\langle m_i \right\rangle_{t-4.5\cdot\tau\le t\le t+5.5\cdot\tau,\,i=1..n}}$$

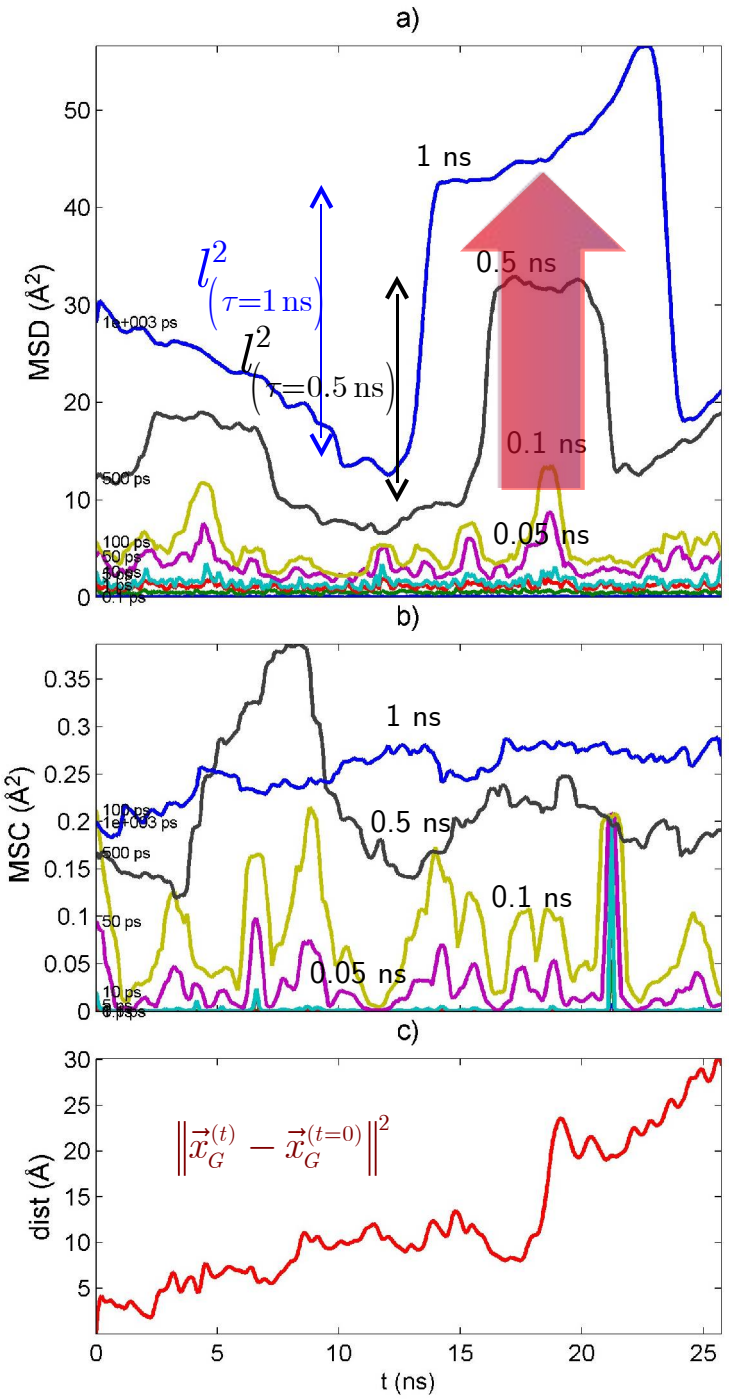
CONTOUR LENGTH FLUCTUATION

2a




residence time (ps·Å$^{-3}$)

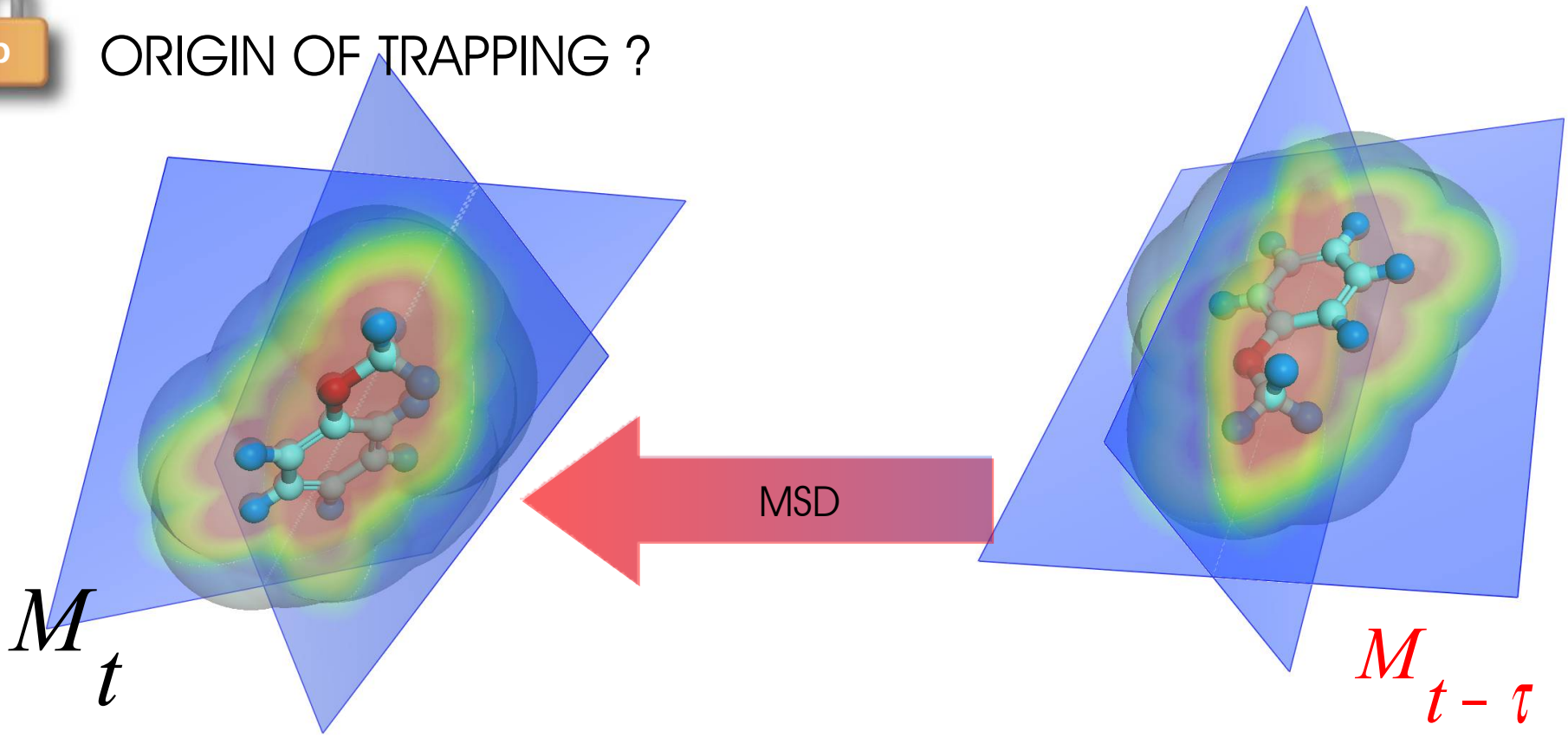
see the videos
http://h29.univ-reims.fr/virtual/MD/anisole16_seq.avi
http://h29.univ-reims.fr/virtual/MD/anisole16_resid_rotation.avi




# HOP IF MSD>MSC

2b

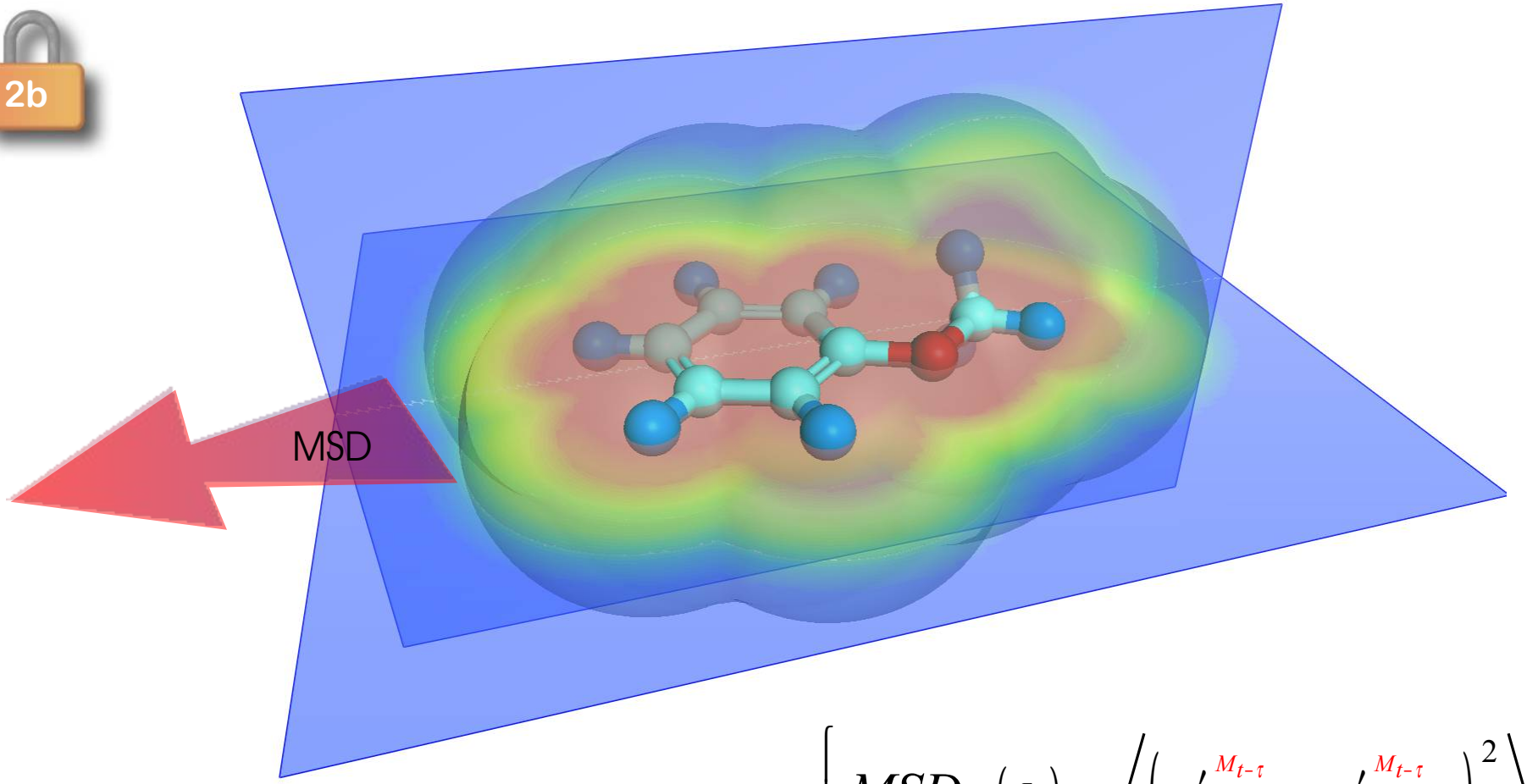
# ORIGIN OF TRAPPING ?




TRAPPRING IS RELATED TO PRIVELEGIED DIRECTIONS OF TRANSLATION
IN THE FRAME OF THE DIFFUSANT ?

HOW TO EXPRESS MSD IN A MOVING-DEFORMABLE FRAME ????

2b

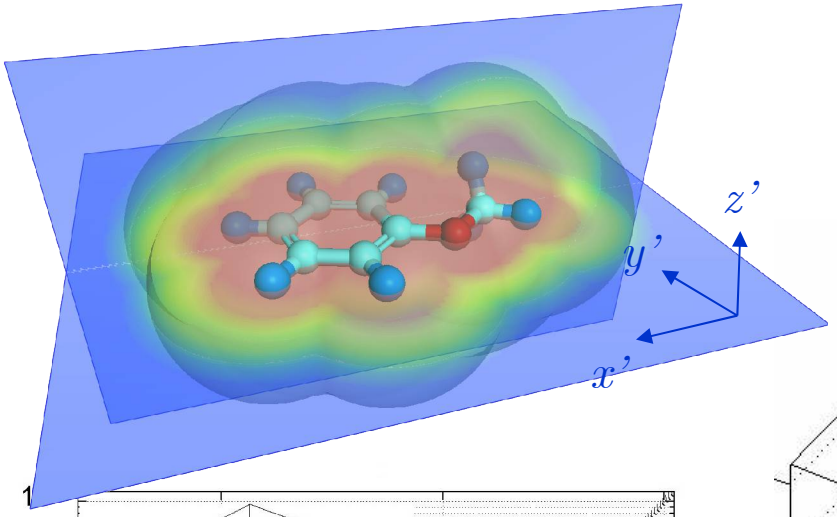


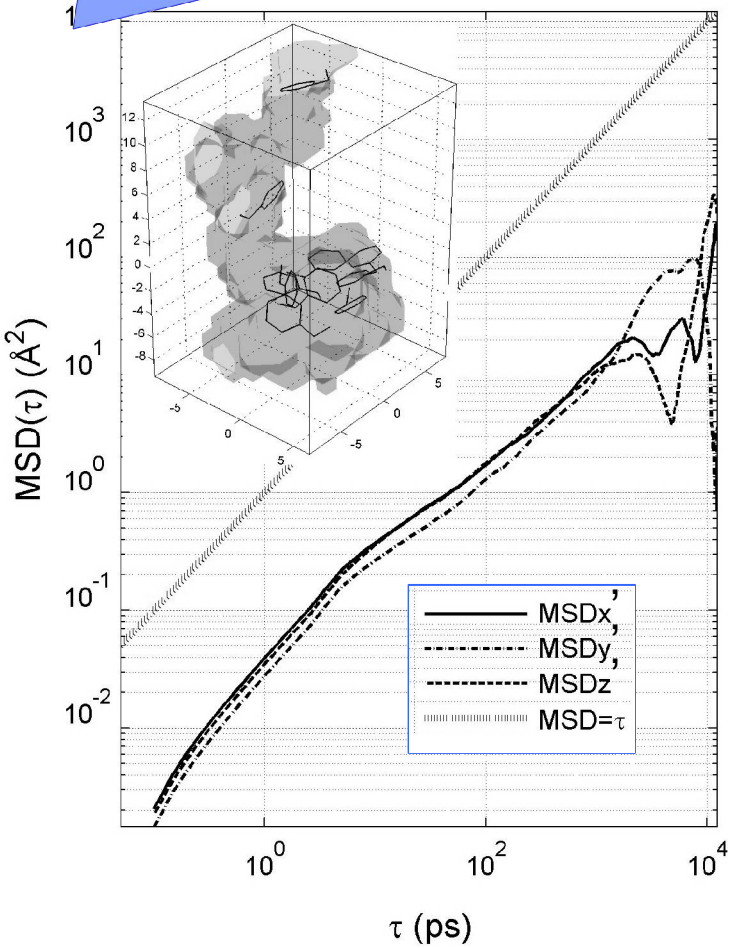

$M_{t-\tau}$ REFERENCE MOLECULAR FRAME
(chosen in the past)

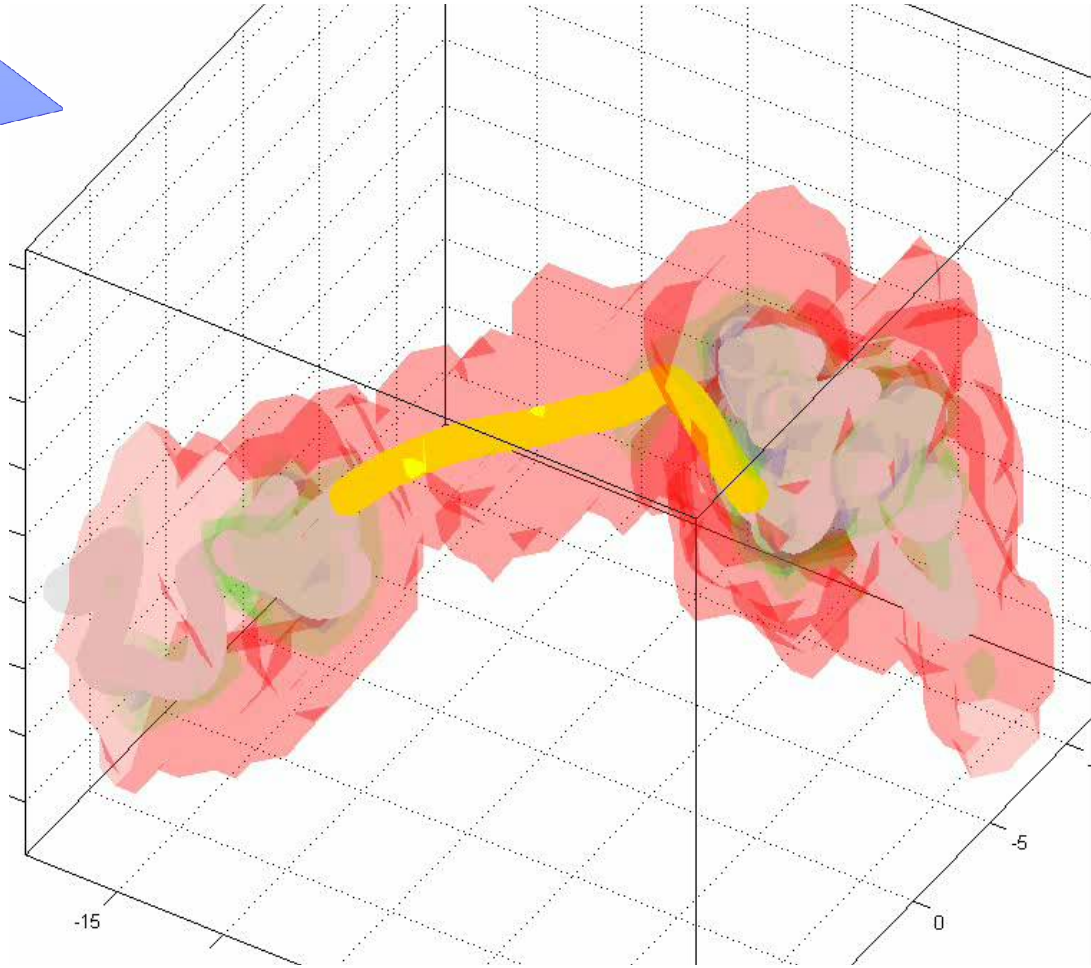
$\forall\ \tau$ : ORTHOGONAL DECOMPOSITION BUT NOT OPTIMAL (TIME CORRELATION)

$$MSD(\tau) = MSD_{x'}(\tau) + MSD_{y'}(\tau) + MSD_{z'}(\tau)$$

$$\begin{cases} MSD_{x'}(\tau) = \left\langle \left( x'^{M_{t-\tau}}_{G,t} - x'^{M_{t-\tau}}_{G,t-\tau} \right)^2 \right\rangle_t \\ MSD_{y'}(\tau) = \left\langle \left( y'^{M_{t-\tau}}_{G,t} - y'^{M_{t-\tau}}_{G,t-\tau} \right)^2 \right\rangle_t \\ MSD_{z'}(\tau) = \left\langle \left( z'^{M_{t-\tau}}_{G,t} - z'^{M_{t-\tau}}_{G,t-\tau} \right)^2 \right\rangle_t \end{cases}$$

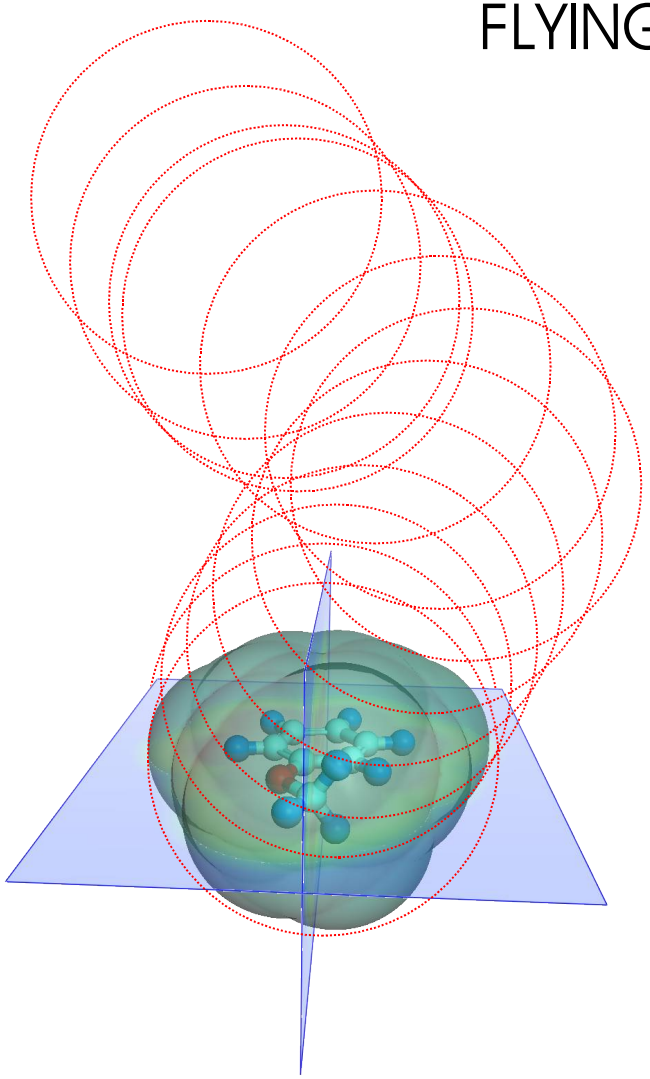



see the video: http://h29.univ-reims.fr/virtual/MD/anisolewww_overview.avi

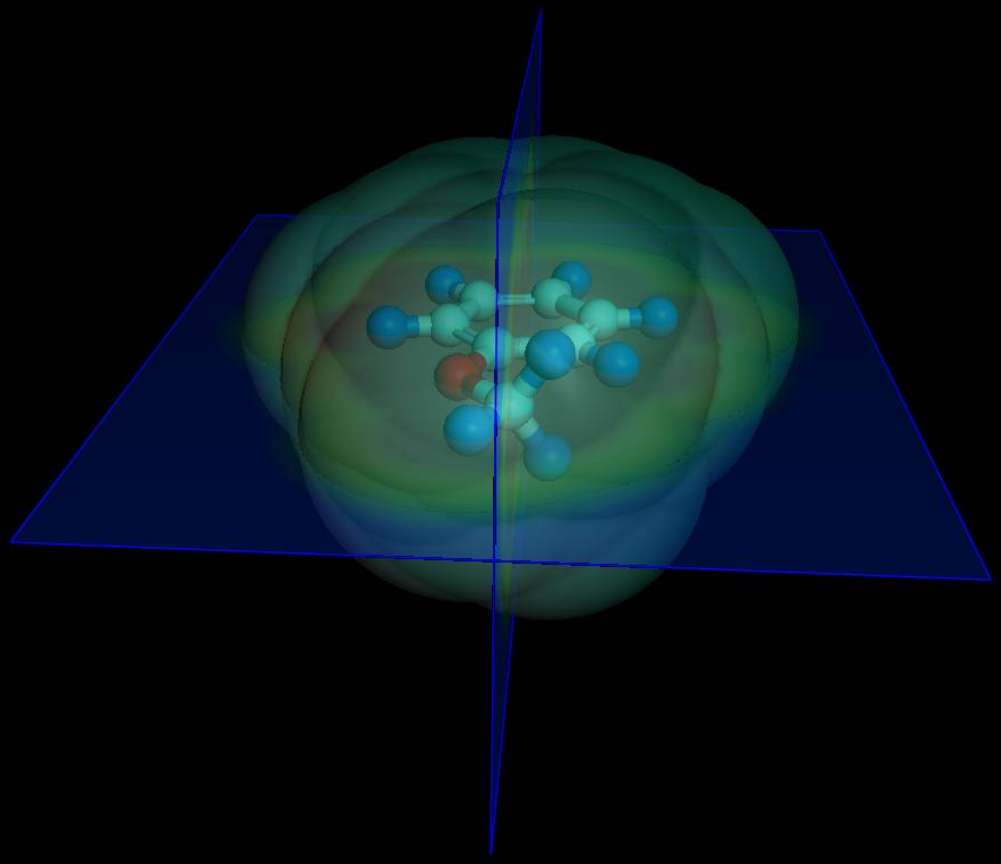
# FLYING WITH ANISOLE IN HDPE (25 ns, smoothed trajectories)



see the video: http://h29.univ-reims.fr/virtual/MD/anisolewww_ontheway.avi

NEXT STEP: TO RELATE THE "TUBE SHAPE" TO THE CONFIGURATIONS OF POLYMER CHAINS

merci pour votre attention



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http://h29.univ-reims.fr