

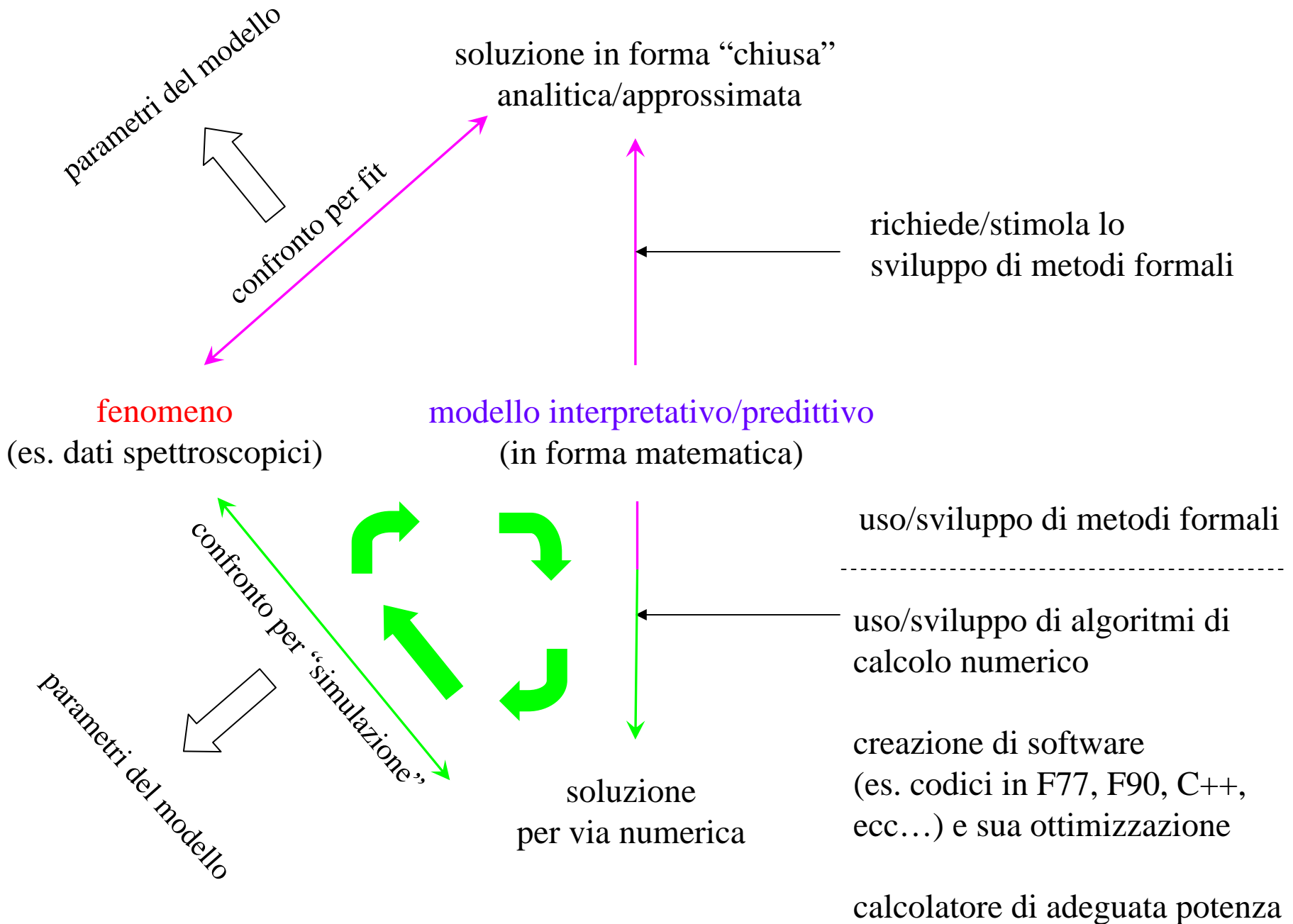
# **Applicazioni dei metodi computazionali in Chimica Fisica**

Opportunità in Chimica Computazionale,  
30 marzo 2007

# Dove entra l'aspetto computazionale in Chimica Fisica?

Consideriamo un aspetto particolare: l'attività del chimico interessato a interpretare dati/descrivere fenomeni sulla base di un modello teorico

[escludiamo ad es. il versante delle simulazioni da Principi Primi, quali tecniche MD, DPD, ecc...]



Da *Introduction to Quantum Mechanics – With Applications to Chemistry,*

L. Pauling, E. B. Wilson

... del 1935 !

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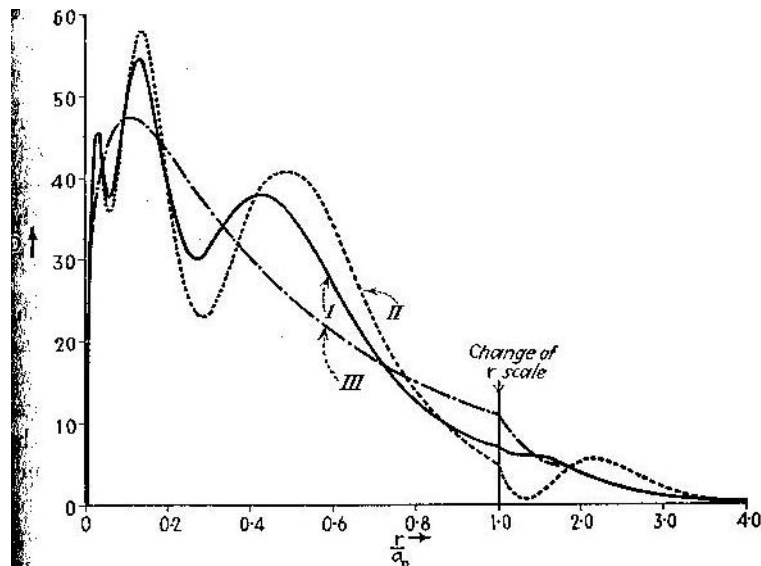


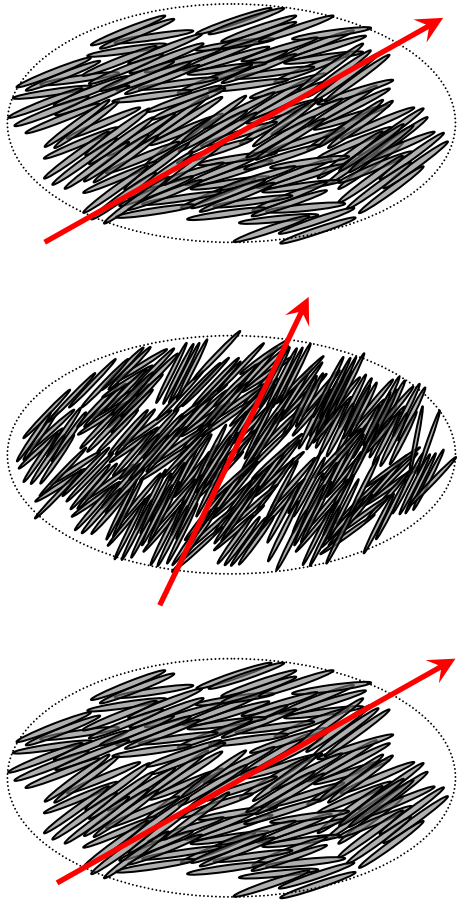
FIG. 32 1. The electron distribution function  $D$  for the normal rubidium atom, as calculated: I, by Hartree's method of the self-consistent field; II, by the screening-constant method; and III, by the Thomas-Fermi statistical method.

CHAPTER IX

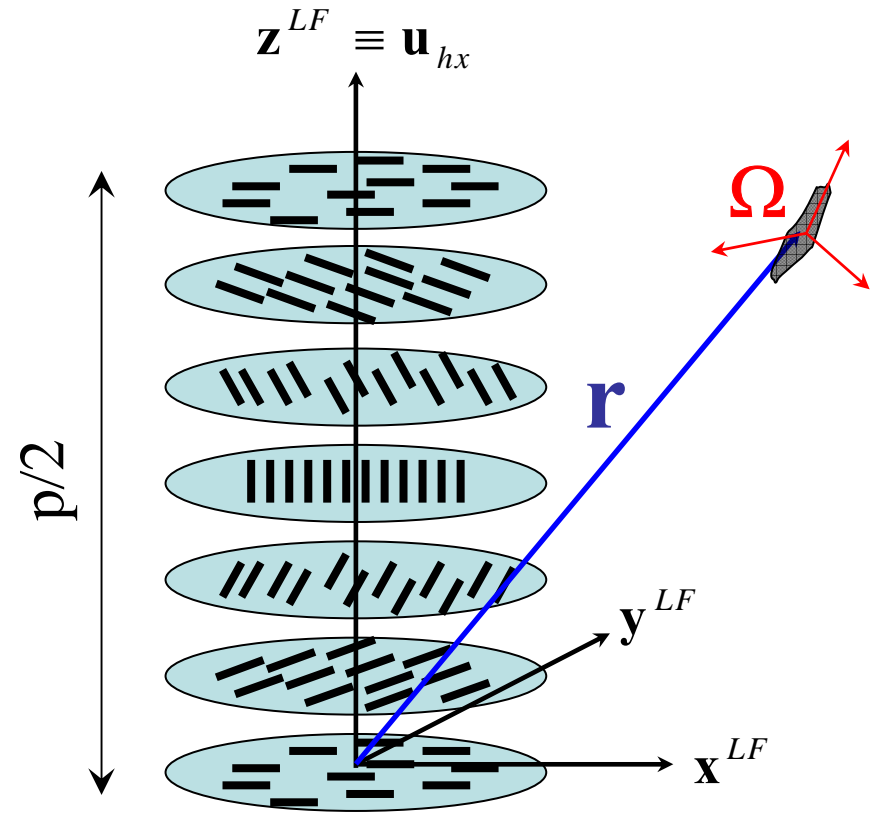
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Un esempio di struttura matematica complessa da trattare  
*necessariamente* per via numerica

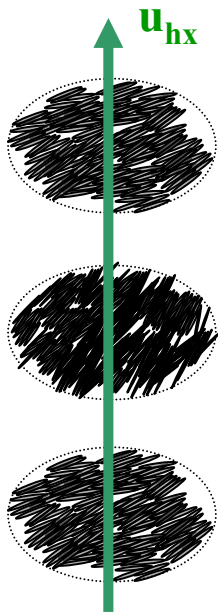


Fase liquido-cristallina  
“colesterica”



$$D_{mt}(\mathbf{u}) = \lim_{t \rightarrow \infty} \frac{\overline{[(\mathbf{r}(t) - \mathbf{r}_0) \cdot \mathbf{u}]^2}}{2t}$$

↑  
direzione di monitoraggio



## Modello:

descrizione della dinamica roto-traslazionale stocastica della singola molecola mediante di diffusione per  $p(\mathbf{r}, \mathbf{\Omega}, t)$  + applicazione al calcolo dell'osservabile specifico

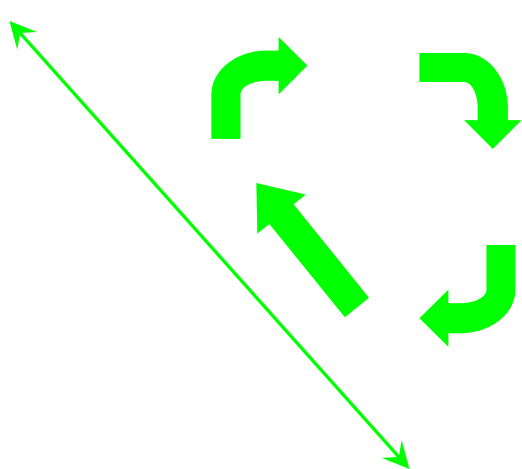
$$D_{mt}(\mathbf{u}_{hx}) = \mathbf{u}_{hx} \cdot \overline{\mathbf{D}_{TT}^{DF}(\mathbf{\Omega}') \mathbf{u}_{hx}} - \int d\mathbf{\Omega}' f(\mathbf{\Omega}') (\Gamma_0')^{-1} f(\mathbf{\Omega}')$$

$$\Gamma_0' = - \begin{pmatrix} 2\pi/p \mathbf{u}_{hx} M_z^{DF} \\ \mathbf{M}^{DF} \end{pmatrix} \cdot \mathbf{D}^{DF}(\mathbf{\Omega}') p_{eq}(\mathbf{\Omega}') \begin{pmatrix} 2\pi/p \mathbf{u}_{hx} M_z^{DF} \\ \mathbf{M}^{DF} \end{pmatrix} p_{eq}(\mathbf{\Omega}')^{-1}$$

$$f(\mathbf{\Omega}') = p_{eq}(\mathbf{\Omega}')^{-1} \mathbf{u}_{hx} \cdot \mathbf{D}_{TR}^{DF}(\mathbf{\Omega}') \mathbf{M}^{DF} p_{eq}(\mathbf{\Omega}') + \frac{2\pi}{p} \mathbf{u}_{hx} \cdot \mathbf{D}_{TT}^{DF}(\mathbf{\Omega}') \mathbf{u}_{hx} p_{eq}(\mathbf{\Omega}')^{-1} M_z^{DF} p_{eq}(\mathbf{\Omega}')$$

**Profilo da generare:**

$D_{mt}(\mathbf{u}_{hx})$  vs. passo elica  $p$

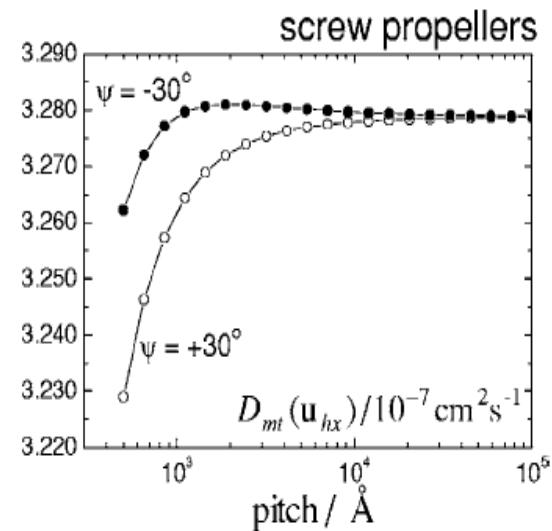
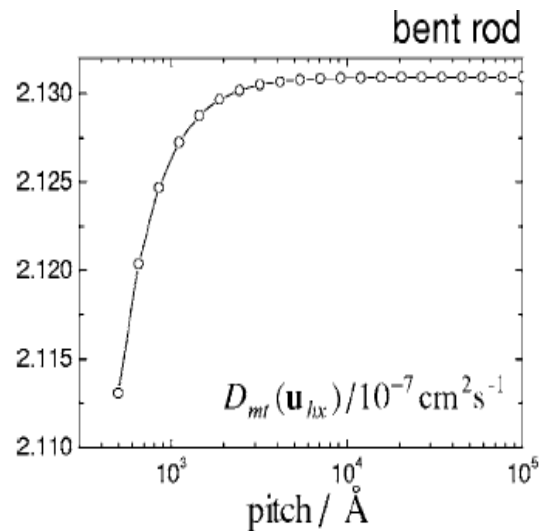
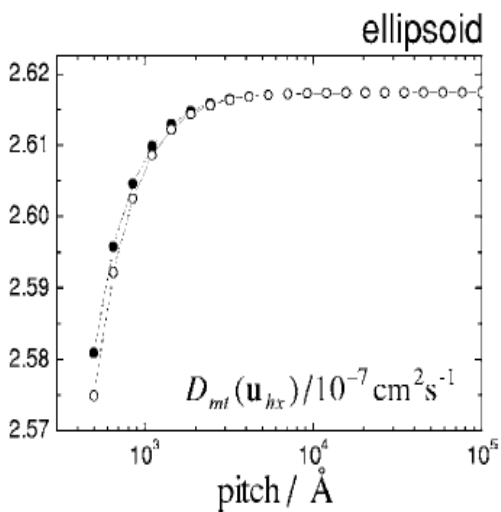
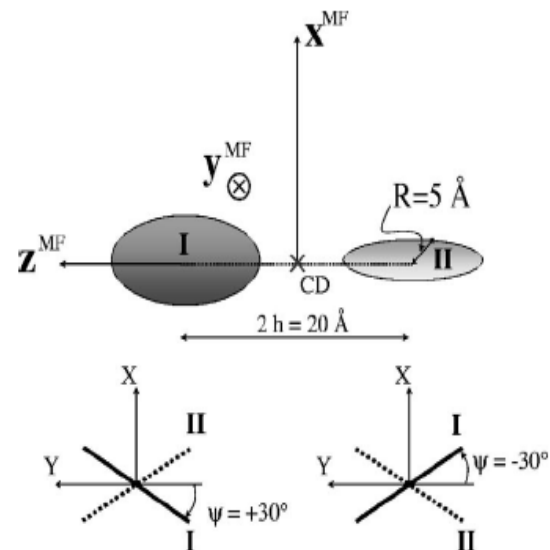
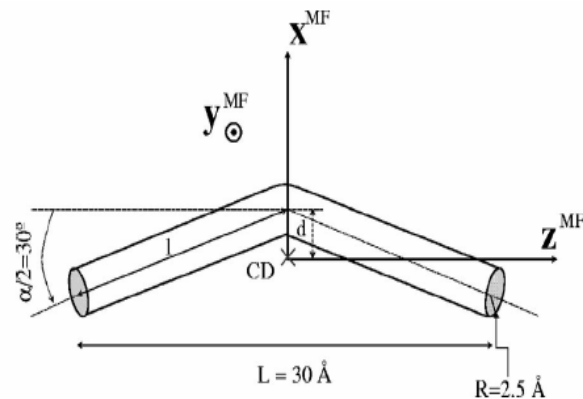
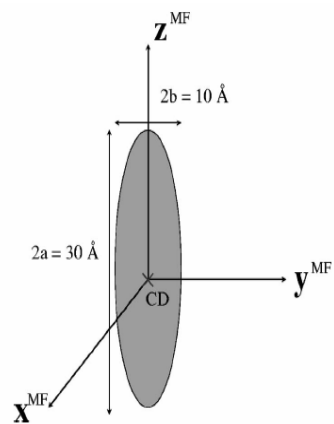


- **Elaborazione** (sviluppo su base di funzioni)

- **Uso/sviluppo di algoritmi** (Lanczos, partizione della matrice inversa, ...)

- **Scrittura di codice** (es. in Fortran)

**Calcolo di  $D_{mt}(\mathbf{u}_{hx})$  per vari parametri di input ...**





Nell'attività del chimico-fisico che si occupa di modelli, l'aspetto computazionale...

- entra come *necessità*, se non è possibile trovare soluzioni chiuse analitiche o approssimate (sufficientemente) accurate.
- stimola la creazione di algoritmi di calcolo trasferibili a problemi diversi.
- si concretizza anche nella creazione di software (che può essere condiviso/commercializzato ...)

... ma attenzione:

- parziale o totale perdita di sintesi “fisica”, se vengono prodotti *direttamente* i risultati numerici!
- la crescente potenza di calcolo a disposizione può limitare lo sviluppo di metodi formali e algoritmi (perché ottimizzarli se posso disporre di un computer più potente?)