Molecular Geometry: from 3D to 5D for Orthogonal Representations of Rigid Motions

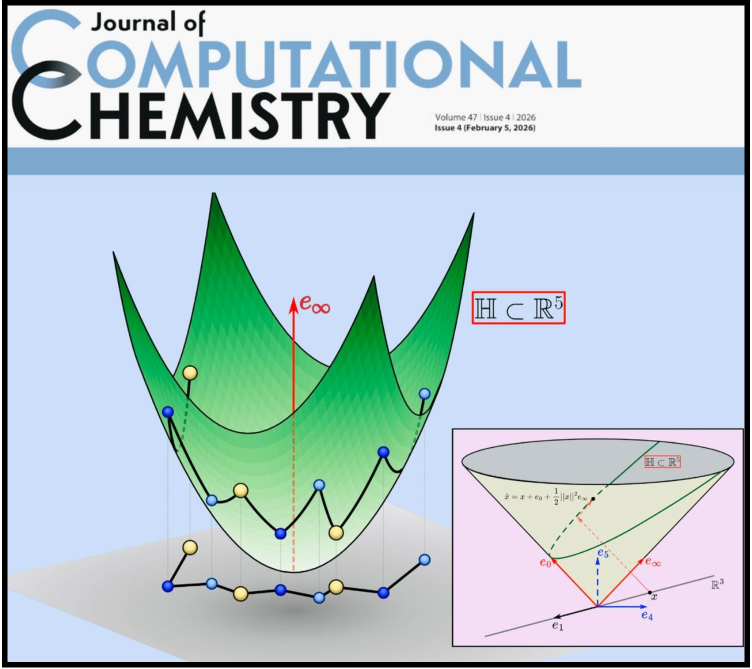
Carlile Lavor

(*joint work with J. Camargo and M. Souza*)

University of Campinas, Brazil

IMECC - UNICAMP

Support: CNPq, FAPESP, ICERM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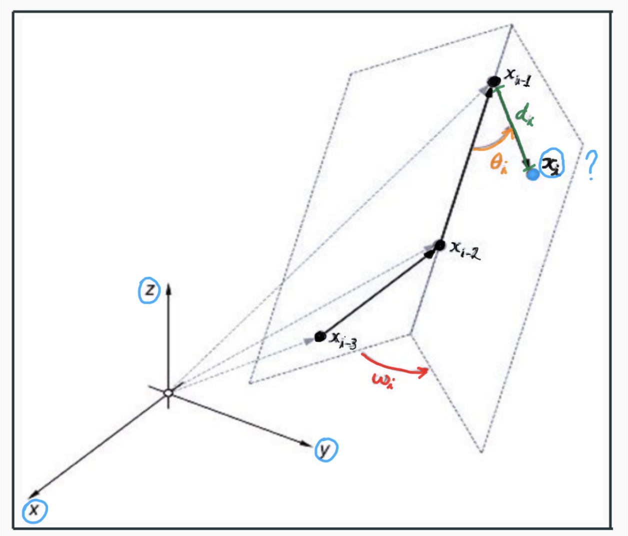
e_∞
$\mathbb{H} \subset \mathbb{R}^5$
$\hat{x} = x + e_0 + \frac{1}{2}||x||^2 e_\infty$
e_0
e_5
e_∞
$\mathbb{R}^3$
x
e_4
e_1



x_{i-1}
d_i
θ_i
x_i
?
x_{i-2}
x_{i-3}
ω_i
z
y
x

- In the homogeneous space:

$$B_{\theta_i} = \begin{bmatrix} -\cos\theta_i & -\sin\theta_i & 0 & 0 \\ \sin\theta_i & -\cos\theta_i & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad B_{\omega_i} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\omega_i & -\sin\omega_i & 0 \\ 0 & \sin\omega_i & \cos\omega_i & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

- For the translation,

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- Combining the matrices,

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- Combining the matrices,

$$
\begin{aligned}
B_i &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\omega_i & -\sin\omega_i & 0 \\ 0 & \sin\omega_i & \cos\omega_i & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} -\cos\theta_i & -\sin\theta_i & 0 & 0 \\ \sin\theta_i & -\cos\theta_i & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & d_i \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \\
&= \begin{bmatrix} -\cos\theta_i & -\sin\theta_i & 0 & -d_i\cos\theta_i \\ \sin\theta_i\cos\omega_i & -\cos\theta_i\cos\omega_i & -\sin\omega_i & d_i\sin\theta_i\cos\omega_i \\ \sin\theta_i\sin\omega_i & -\cos\theta_i\sin\omega_i & \cos\omega_i & d_i\sin\theta_i\sin\omega_i \\ 0 & 0 & 0 & 1 \end{bmatrix}.
\end{aligned}
$$

- With $d_1 = \omega_1 = \omega_2 = \omega_3 = 0$ and $\theta_1 = \theta_2 = \pi$, we get [1]

$$x_1 = B_1 e_4 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}, \qquad x_2 = (B_1 B_2) e_4 = \begin{bmatrix} d_2 \\ 0 \\ 0 \\ 1 \end{bmatrix},$$

$$x_3 = (B_1 B_2 B_3) e_4 = \begin{bmatrix} (d_2 - d_3 \cos\theta_3) \\ d_3 \sin\theta_3 \\ 0 \\ 1 \end{bmatrix},$$

$$x_i = (B_1 B_2 B_3 \cdots B_i) e_4,$$

$i = 4, \ldots, n$ and $e_4 = (0, 0, 0, 1)^t$.

[1] Thompson (1967)

- Let us write

$$B_{[i,j]} = \prod_{k=i}^{j} B_k$$

and calculate the Euclidean distance $r_{i,j}$ $(x_i, x_j \in \mathbb{R}^4)$:

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  - In $\mathbb{R}^{3\times 3}$:

$$r_{i,j} = \left\| \left(d_{i+1} I + \sum_{s=i+2}^{j} d_s B_{[i+2,s]} \right) e_1 \right\|.$$

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The Conformal Model

- In the Homogeneous Model,

$$H(x) = \underline{x + e_4} =$$

[2] Dress and Havel (1993)
[3] Li, Hestenes, and Rockwood (2001)
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- In the Homogeneous Model,

$$H(x) = \underline{x + e_4} = \begin{bmatrix} x \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} x \\ 1 \end{bmatrix},$$

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$$C(x) = x + e_0 + (?)e_\infty =$$

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$$C(x) = x + e_0 + (?)e_\infty = \begin{bmatrix} x \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} + \left(\frac{1}{2}\|x\|^2\right) \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} =$$

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$x \in \mathbb{R}^3$, $C(x) \in \mathbb{R}^5$.

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$x \in \mathbb{R}^3$.

- In our particular case,

$$
U = \begin{bmatrix} A & b & 0 \\ 0 & 1 & 0 \\ b^t A & \frac{\|b\|^2}{2} & 1 \end{bmatrix}
= \begin{bmatrix} -\cos\theta_i & -\sin\theta_i & 0 & -d_i\cos\theta_i & 0 \\ \sin\theta_i\cos\omega_i & -\cos\theta_i\cos\omega_i & -\sin\omega_i & d_i\sin\theta_i\cos\omega_i & 0 \\ \sin\theta_i\sin\omega_i & -\cos\theta_i\sin\omega_i & \cos\omega_i & d_i\sin\theta_i\sin\omega_i & 0 \\ 0 & 0 & 0 & 1 & 0 \\ d_i & 0 & 0 & \frac{d_i^2}{2} & 1 \end{bmatrix}.
$$

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$$r_{i,j} \neq \|(x_j - x_i)\|,$$

$x_i, x_j \in \mathbb{R}^5$.

- PROBLEM: How to define a bijection between $\mathbb{R}^3$ and a subset $H \subset \mathbb{R}^5$, in such a way that isometries in $\mathbb{R}^3$ can be represented orthogonally in $\mathbb{R}^5$?

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Points in 3D space $\rightarrow$ vectors in $\mathbb{R}^5$ with zero norm

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Points in 3D space $\rightarrow$ vectors in $\mathbb{R}^5$ with zero norm (NULL VECTORS)

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$\underline{x = x_1 e_1 + x_2 e_2 + x_3 e_3}$ and $\{e_1, e_2, e_3, e_4, e_5\}$ is an orthogonal basis in $\mathbb{R}^5$.

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- From the algebraic properties of the inner product in $\mathbb{R}^5$,

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$$\underline{\hat{x} \cdot \hat{x} = 0} \implies x_4^2 (e_4 \cdot e_4) + x_5^2 (e_5 \cdot e_5) = -\|x\|^2.$$

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- Assuming

$$(x \neq 0 \quad \textit{and} \quad \|e_4\| = 1) \implies$$

- Choosing a basis in $\mathbb{R}^5$:

$$\hat{x} = x + x_4 e_4 + x_5 e_5,$$

$x = x_1 e_1 + x_2 e_2 + x_3 e_3$ and $\{e_1, e_2, e_3, e_4, e_5\}$ is an orthogonal basis in $\mathbb{R}^5$.

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- As a consequence,

$$\hat{x}\cdot\hat{y} = \left(x + e_0 + \frac{1}{2}\|x\|^2 e_\infty\right)\cdot\left(y + e_0 + \frac{1}{2}\|y\|^2 e_\infty\right) = -\frac{1}{2}\|x-y\|^2.$$

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$$\hat{x} \cdot \hat{y} = \begin{bmatrix} x_1 & x_2 & x_3 & x_0 & x_\infty \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_0 \\ y_\infty \end{bmatrix} = \hat{x}^t I_c \hat{y},$$

where

$$I_c = \begin{bmatrix} I & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix}$$

and $I \in \mathbb{R}^{3 \times 3}$.

- Considering

$$U = \begin{bmatrix} A & b & 0 \\ 0 & 1 & 0 \\ b^t A & \frac{\|b\|^2}{2} & 1 \end{bmatrix},$$

it is easy to check that

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and, in turn,

$$(U\hat{x}) \cdot (U\hat{y}) = (U\hat{x})^t I_c (U\hat{y}) = \hat{x}^t (U^t I_c U)\hat{y} = \hat{x} \cdot \hat{y},$$

for all $x, y \in \mathbb{R}^3$.

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$$B_k = \begin{bmatrix} -\cos\theta_k & -\sin\theta_k & 0 & -d_k\cos\theta_k & 0 \\ \sin\theta_k\cos\omega_k & -\cos\theta_k\cos\omega_k & -\sin\omega_k & d_k\sin\theta_k\cos\omega_k & 0 \\ \sin\theta_k\sin\omega_k & -\cos\theta_k\sin\omega_k & \cos\omega_k & d_k\sin\theta_k\sin\omega_k & 0 \\ 0 & 0 & 0 & 1 & 0 \\ d_k & 0 & 0 & \frac{d_k^2}{2} & 1 \end{bmatrix}.$$

- First, let's write $(i < j)$

$$B_{[i+1,j]} = \prod_{k=i+1}^{j} B_k$$

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- That is,

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$$r_{i,j} = \left\| \left(d_{i+1} I + \sum_{s=i+2}^{j} d_s B_{[i+2,s]} \right) e_1 \right\|,$$

$e_1 \in \mathbb{R}^3$.

Number of operations to calcule $r_{i,j}$

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Model	Number of Operations
Euclidean	$55(j-i)-97$
Homogeneous	$35(j-i)-25$
Conformal	$28(j-i)-45$

Main References

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Thank you!