DT-MRI Images : Estimation, Regularization and Application

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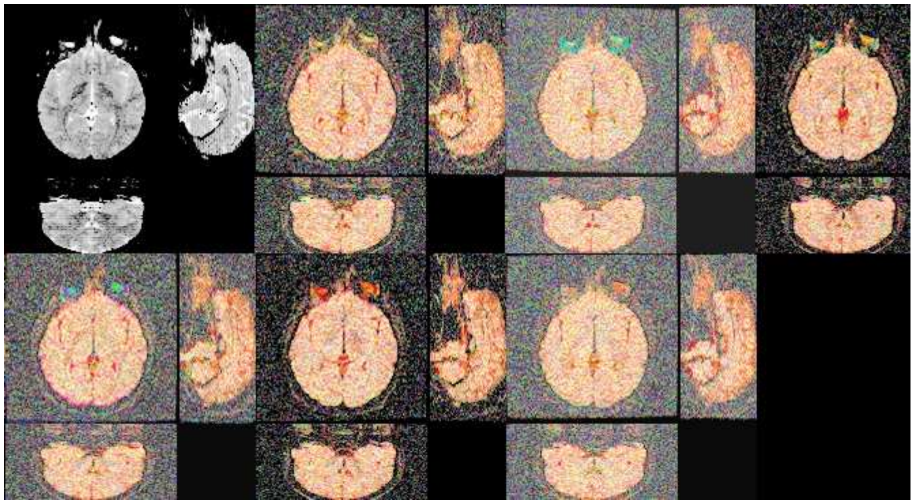
Abstract. Diffusion-Tensor MRI is a technique allowing the measurement of the *water molecule motion* in the tissues fibers, by the mean of rendering multiple MRI images under different oriented magnetic fields. This large set of raw data is then further estimated into a *volume of diffusion tensors* (i.e. 3×3 symmetric and positive-definite matrices) that describe through their spectral elements, the diffusivities and the main directions of the tissues fibers. We address two crucial issues encountered for this process : diffusion tensor *estimation* and *regularization*. After a review on existing algorithms, we propose alternative variational formalisms that lead to new and improved results, thanks to the introduction of important tensor constraint priors (positivity, symmetry) in the considered schemes. We finally illustrate how our set of techniques can be applied to enhance fiber tracking in the white matter of the brain.

1 Introduction

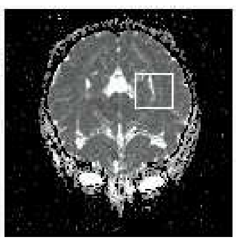
The recent introduction of DT-MRI (Diffusion Tensor Magnetic Resonance Imaging) has raised a strong interest in the medical imaging community [14]. This non-invasive 3D modality consists in measuring the water molecule motion within the tissues, using magnetic resonance techniques. It is based on the rendering of multiple raw MRI volumes $S_k : \Omega \subset \mathbb{R}^3 \rightarrow \mathbb{R}$ using pulse sequences with several gradient directions and magnitudes (at least 6 noncolinear directions are necessary). An additional image S_0 is also measured without preferred gradient direction (Fig.1a). These S_k may be quite noisy, due to the high speed needed for these multiple MRI acquisitions. This large set $\{S_k, k = 0...n\}$ of raw volumes is then estimated into a corresponding volume $\mathbf{T} : \Omega \subset \mathbb{R}^3 \rightarrow \mathrm{P}(3)$ of Diffusion Tensors (i.e 3x3 symmetric and positive-definite matrices) that describe through their spectral elements, the main diffusivities $\lambda_1, \lambda_2, \lambda_3$ (with $\lambda_1 \geq \lambda_2 \geq \lambda_3$) and the corresponding principal orthogonal directions $\mathbf{u}^{[1]}$,$\mathbf{u}^{[2]}$,$\mathbf{u}^{[3]}$ of the water molecule diffusion in tissues such as bones, muscles and white matter of the brain (Fig.1b).

$$\forall x, y, z \in \Omega, \qquad \mathbf{T}(x, y, z) = \lambda_1 \mathbf{u}^{[1]} \mathbf{u}^{[1]^T} + \lambda_2 \mathbf{u}^{[2]} \mathbf{v}^{[2]^T} + \lambda_3 \mathbf{u}^{[3]} \mathbf{w}^{[3]^T}$$

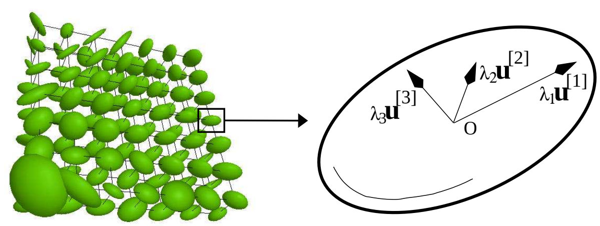
Depending on the characteristics of the tissue, the diffusion (and then the es-



(a) Measured raw acquisitions S_k $(k = 0 \ldots 6)$



(b1) Mean diffusivity = $\frac{1}{3}(\lambda_1 + \lambda_2 + \lambda_3)$



(b2) Part of the estimated tensor field $\mathbf{T}$, represented with 3D ellipsoids.

Fig. 1. Principle of DT-MRI Imaging

timated tensors) can be isotropic (for instance in the areas with fluids such in the CSF filled ventricles) or anisotropic as in the white matter of the brain where the diffusion is mainly performed in the direction of the neuron fibers [15, 30]. DT-MRI is then particularly well adapted to study the brain connectivities, by tracking the fiber directions given pointwise by the principal eigenvector $\mathbf{u}^{[1]}(x, y, z)$ of the tensor $\mathbf{T}(x, y, z)$.
Actually, retrieving the fiber bundles from the raw images S_k involves two subjacent processes : First the *estimation part*, which estimates the diffusion tensors as gaussian models of the water diffusion, directly from the raw data S_k. Then, as the obtained tensor field $\mathbf{T}$ may be noisy, a specific *regularization process* can be necessary to improve the result.
Here we propose a survey of the related methods in the literature and introduce new variational frameworks that take important tensor structural constraints into account for these estimation and regularization steps. We highlight the different advantages of our formulations over the previous ones and we illustrate how our set of approaches can be used to obtain fiber tracking results from synthetic and real DT-MRI datasets of the brain.

2 Diffusion Tensor Estimation

2.1 Review of existing methods

The estimation process gathers the informations given by the multiple physical measures S_k of the diffusion MRI into a field of 3×3 symmetric matrices $\mathbf{T}$ which represent gaussian models of the water molecule diffusion. This link is given through the Stejskal-Tanner equation [21] :

$$\forall (x,y,z) \in \Omega, \qquad S_{k_{(x,y,z)}} = S_{0_{(x,y,z)}} \; e^{-b g_k^T \mathbf{T}_{(x,y,z)} g_k} \tag{1}$$

where the b-factor is a constant, depending on the acquisition parameters and $g_k \in \mathbb{R}^3$ is a vector representing the pulse gradient magnitude ($\|g_k\|$) and direction ($g_k/\|g_k\|$) used for the acquisition of the image S_k. Classical methods for computing the tensor $\mathbf{T}$ from the images S_k have been already proposed in the literature :

- **Direct tensor estimation :** proposed by Westin-Maier [29], this method lies on the decomposition of $\mathbf{T}$ in an orthonormal tensor basis $\tilde{g_k}\tilde{g_k}^T$ (with $\tilde{g_k} = g_k/\|g_k\|$ and $k = 1..6$). The 6 coordinates of $\mathbf{T}$ in this basis (which are *dot products* in tensor space), naturally appear in eq.(1), and can then be retrieved :

$$\mathbf{T} = \sum_{k=1}^{6} < \mathbf{T}, \tilde{g_k}\tilde{g_k}^T > \; \tilde{g_k}\tilde{g_k}^T = \sum_{k=1}^{6} \frac{1}{b\|g_k\|^2} \ln\left(\frac{S_0}{S_k}\right) \tilde{g_k}\tilde{g_k}^T \tag{2}$$

It particularly means that only 7 raw images $S_0, ..., S_6$ are used to estimate the diffusion tensor field $\mathbf{T}$. As illustrated with the synthetic example in Fig.2, this low number of images may be not sufficient for a robust estimation of $\mathbf{T}$, particularly if the S_k are corrupted with a high variance noise.

- **Least square estimation**, is nowadays the most classical method used for diffusion tensor estimation since it can use all the available raw volumes S_k (see for instance [3, 18]). The tensors $\mathbf{T}$ are estimated by minimizing the following least square criterion,

$$\min_{\mathbf{T} \in \mathcal{M}_3} \quad \sum_{k=1}^{n} \left(\frac{1}{b} \ln\left(\frac{S_0}{S_k}\right) - g_k^T \mathbf{T} g_k \right)^2 \tag{3}$$

which leads to the resolution of an overconstrained system $\mathbf{Ax} = \boldsymbol{\mathcal{B}}$ with a pseudo-inverse solution $\mathbf{x} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T \; \boldsymbol{\mathcal{B}}$ (where $\mathbf{x}$ is a vector containing the six unknown coefficients $T_{xx}, T_{xy}, T_{xz}, T_{yy}, T_{yz}, T_{zz}$ of $\mathbf{T}$). The least square method generally gives better results for noisy datasets, since all the S_k (usually $n >> 7$) are used in the estimation process.

Note that no one of both methods takes any prior positive-definite constraints of the tensors $\mathbf{T}$ into account. Nothing prevents the computation of negative tensors (i.e with negative diffusivities). Practically, one has to check the tensor positivity after estimation, and reproject the negative tensors into the positive tensor space. This is generally done by forcing the negative eigenvalues of the tensors to zero : $\forall(x,y,z)\in\Omega,\quad \tilde{\mathbf{T}}=\tilde{\lambda_1}\mathbf{u}\mathbf{u}^T+\tilde{\lambda_2}\mathbf{v}\mathbf{v}^T+\tilde{\lambda_3}\mathbf{w}\mathbf{w}^T$, with $\tilde{\lambda_i}=\max(0,\lambda_i)$ (This projection minimizes the Mahalanobis distance between $\mathbf{T}$ and $\tilde{\mathbf{T}}$). Note also that both estimation methods are purely *pointwise* : no spatial interactions are considered during the estimation.

2.2 A robust variational estimation

In order to avoid these important drawbacks, we propose a variational approach that estimates the tensor field $\mathbf{T}$ from the raw volumes S_k while introducing important priors on the *tensor positivity* and *regularity*. Our idea is based on the *positive-constrained minimization* of a least-square criterion, coupled with an anisotropic regularization term :

$$\min_{\mathbf{T}\in\mathrm{P}(3)}\int_\Omega\sum_{k=1}^{n}\left(\frac{1}{b}\ln\left(\frac{S_0}{S_k}\right)-g_k^T\mathbf{T}g_k\right)^2+\alpha\,\phi(\|\nabla\mathbf{T}\|)\,d\Omega \qquad (4)$$

where b is the constant factor depending on the acquisition parameters, g_k is the pulse gradient vector associated to the image S_k, $\alpha\in\mathbb{R}$ is a user-defined regularization weight and $\phi:\mathbb{R}\to\mathbb{R}$ is a regularizing ϕ-functional that measures the tensor field variations through the operator $\|\nabla\mathbf{T}\|=(\sum_{i,j}\|\nabla T_{i,j}\|^2)^{\frac{1}{2}}$. The minimization is then performed by a gradient descent (iterative method), *on the constrained space* P(3), representing the set of 3×3 symmetric and positive-definite matrices. Following our previous theoretical work on constrained matrix flows [9], the matrix-valued PDE minimizing (4) in P(3) with its natural metric is :

$$\begin{cases}\mathbf{T}_{(t=0)}=\mathbf{Id}\\[2ex] \dfrac{\partial\mathbf{T}}{\partial t}=-((\mathbf{G}+\mathbf{G}^T)\mathbf{T}^2+\mathbf{T}^2(\mathbf{G}+\mathbf{G}^T))\end{cases} \qquad (5)$$

where $\mathbf{Id}$ is the 3×3 identity matrix and $\mathbf{G}=(G_{i,j})$ is the matrix defined as :

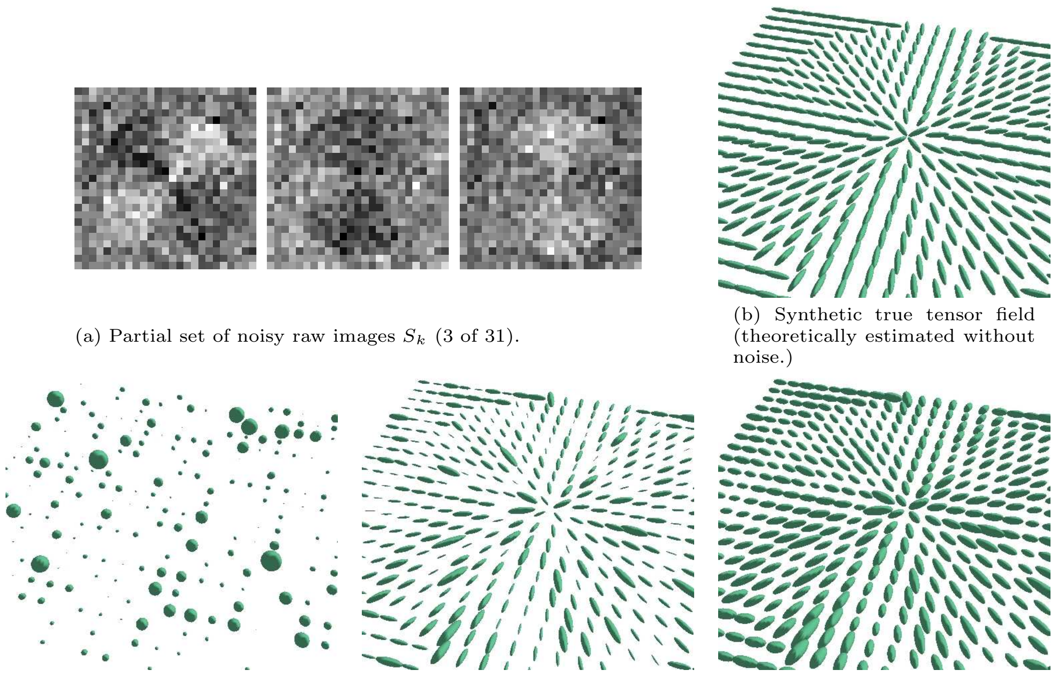
$$G_{i,j}=\sum_{k=1}^{n}\left(\frac{1}{b}\ln\left(\frac{S_0}{S_k}\right)-g_k^T\mathbf{T}g_k\right)\,\left(g_kg_k^T\right)_{i,j}-\frac{\alpha}{2}\,\mathrm{div}\left(\frac{\phi'(\|\nabla\mathbf{T}\|)}{\|\nabla\mathbf{T}\|}\nabla T_{i,j}\right)$$

Eq.(5) ensures the positive-definiteness of the tensors $\mathbf{T}$ for each iteration of the estimation process. Moreover, the regularization term α introduces some spatial regularity on the estimating tensor field, *while preserving important physiological discontinuities* thanks to the anisotropic behavior of the ϕ-function regularization formulation (as described in the broad literature on anisotropic smoothing with PDE's, see for instance [1, 20, 23, 28] and references therein).

Moreover, a specific reprojection-free numerical scheme based on matrix exponentials can be used for this flow lying in P(3), as described in [9] :

$$\mathbf{T}_{(t+dt)}=\mathbf{A}^T\mathbf{T}_{(t)}\mathbf{A}\quad\text{with}\quad\mathbf{A}=\exp\left(-\mathbf{T}_{(t)}(\mathbf{G}+\mathbf{G}^T)dt\right)$$

This scheme preserves numerically the positive-definiteness of the estimating tensors. The algorithm starts then at $t = 0$ with a field of *isotropic tensors* that are iteratively evolving in P(3) until their shapes fit the measured data S_k with respect to the Stejskal-Tanner model eq.(1) and the positivity and regularity constraints. The respect of these natural diffusion tensor constraints has a large interest for DT-MRI, and leads to more accurate results than with classical methods. It is illustrated on Fig.2, with the estimation of a synthetic field from noisy images S_k.



(a) Partial set of noisy raw images S_k (3 of 31).

(b) Synthetic true tensor field (theoretically estimated without noise.)

(c) Direct estimation of the S_k with 7 non-colinear images,eq.(2).

(d) Least square estimation of the S_k, eq.(3) with 41 images.

(e) Our variational estimation method eq.(5), using positivity and regularity constraints.

Fig. 2. DT-MRI Estimation : Comparison of our variational method for diffusion tensor estimation from noisy raw volumes S_k, with classical estimation techniques.

In Fig.2d, notice the presence of false estimations, i.e negative estimated tensors that needed to be reprojected into the positive tensor space, and that appears very thin (at least one eigenvalue has been set to zero). These false estimations naturally disappear with our constrained method (Fig.2e). Raw data that tends to transform the positive tensors into negative ones are intrinsically ignored by the algorithm, thanks to the tensor positivity and regularity a-priori.

3 DT-MRI Regularization

During MRI image acquisition, the raw images may be corrupted by noise and specific regularization methods are needed to obtain more coherent diffusion tensor maps. Recently, several methods have been proposed in the literature to deal with this important problem. These methods can be divided into two classes.

3.1 Non-spectral regularization methods

- **Smoothing the raw images S_k :** Vemuri-Chen-etal, proposed a scheme in [27] that regularizes directly the raw images S_k *before tensor estimation*, by using a PDE-based regularization scheme that takes the coupling between the S_k into account.

$$\forall k = 0...n, \qquad \frac{\partial S_k}{\partial t} = \text{div}\left(\frac{g(\lambda_+, \lambda_-)}{\|\nabla S_k\|}\nabla S_k\right) - \mu(S_k - S_{k_{(t=0)}})$$

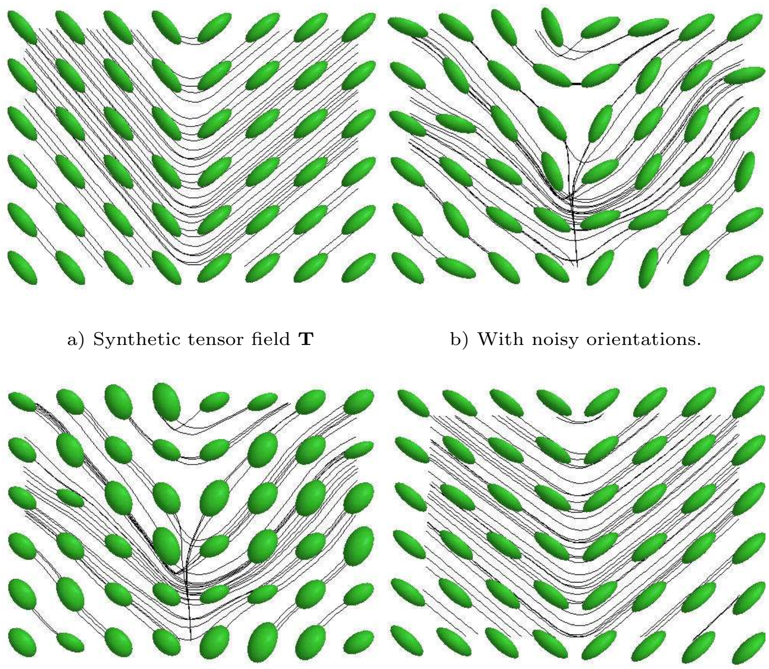
The coupling here is done through the two eigenvalues $\lambda_\pm$ coming from a first estimation of the tensors $\mathbf{T}$, with a least square method. After regularization, the tensor field is re-estimated from the regularized version $\tilde{S}_k$, resulting in a smoother version of $\mathbf{T}$.

- **Direct matrix smoothing :** Another approach, proposed in [5, 9] is to estimate the tensor field $\mathbf{T} \ : \Omega \rightarrow \mathrm{P}(n)$ from the S_k, then consider it as a multi-valued image with 6 components (i.e the number of different coefficients in a 3×3 matrix). This multivalued image is then processed with classic vector-valued diffusion PDE's (such as in [13, 20, 22, 25, 26]).

$$\frac{\partial T_{i,j}}{\partial t} = \text{div}\left(\mathbf{D}\nabla T_(i,j)\right) \tag{6}$$

where $\mathbf{D}$ is a 3×3 diffusion tensor that drives the regularization process. This tensor $\mathbf{D}$ generally depends on $\mathbf{T}$ and its spatial derivatives. Moreover, the method proposed in [9] ensures the tensor positivity constraint, in a theoretical way, as well as the respect of a natural metric in the positive tensor space.

- **Drawbacks :** By definition, non-spectral methods cannot have a direct control on the spectral elements of the tensors, which are however the relevant features that characterizes the biological tissues. During non-spectral regularization processes, tensor orientations and diffusivities are smoothed *at the same time*. Unfortunately, tensor diffusivities are regularizing faster than tensor orientation, resulting in an eigenvalue swelling effect for long time regularization (Fig.3). Then, a high risk of losing tensor orientation occurs : the tensors are quite fastly converging to *identity matrices*.



a) Synthetic tensor field $\mathbf{T}$ b) With noisy orientations.

c) Direct matrix diffusion (eq.(6)) d) Spectral regularization (section.3.2)

Fig. 3. Spectral versus Non-Spectral regularization methods.

3.2 Spectral regularization methods

The idea behind spectral regularization methods of diffusion tensor fields lies in the separate (but eventually coupled) regularization of the tensor *diffusivities* λ_l (three eigenvalues, $l = 1..3$) and *orientations* $\mathbf{u}^{[l]}$ (three eigenvectors). Actually, the tensors are decomposed into :

$$\mathbf{T} = \mathbf{U}\ \boldsymbol{\Gamma}\ \mathbf{U}^T \qquad \text{where} \quad \boldsymbol{\Gamma} = \text{diag}(\lambda_1, \lambda_2, \lambda_3) \quad \text{and} \quad \mathbf{U} = \left(\ \mathbf{u}^{[1]} \mid \mathbf{u}^{[2]} \mid \mathbf{u}^{[3]}\ \right)$$

This is for instance the matter of the papers [9, 11, 24]. Indeed, the undesired eigenvalues swelling effect can be avoided by regularizing tensor eigenvalues more slowly than tensor orientations. The smoothing process must also consider the tensor constraints (positivity, symmetry) *in the spectral space*, which are expressed as :

$$\begin{cases} \text{Positivity : } \forall l \qquad \lambda_l \geq 0 \\ \\ \text{Symmetry : } \forall k, l, \qquad \mathbf{u}^{[k]}.\mathbf{u}^{[l]} = \delta_{k,l} \qquad (\mathbf{U} \text{ is an orthogonal matrix}) \end{cases} \tag{7}$$

Different methods have been already propose to regularize these two spectral fields :

- Regularization of the tensor diffusivities : Tensor diffusivities are considered as a multi-channel image, with 3 components $(\lambda_1, \lambda_2, \lambda_3)$ and can then be regularized with anisotropic PDE schemes, already proposed in the literature for this kind of image [13, 20, 22, 23, 25, 26]). Moreover, one can easily drive the diffusivities regularization by considering specific DT-MRI indices, like mean diffusivity, fractional anisotropy, etc. (Fig.4).

$$\frac{\partial \lambda_l}{\partial t} = \operatorname{div}\left(\mathbf{D}(\lambda_i, FA, VR, ...)\, \nabla \lambda_l\right) \tag{8}$$

The positivity constraint of theses eigenvalues λ_l is simply ensured by using a scheme that satisfies the *maximum and minimum principle* [2].

- Regularization of the tensor orientations : The difficult part of the spectral regularization methods come from the regularization of the tensor orientations. In [11, 24], the authors propose to regularize only the field of the principal direction $\mathbf{u}^{[1]}$, using a modified version of the norm constrained TV-regularization, as defined in [7]. Then, the two other tensor directions $\mathbf{u}^{[2]}$ and $\mathbf{u}^{[3]}$ are rebuild from the original noisy tensor orientation $\mathbf{U}$ and the regularized principal direction $\tilde{\mathbf{u}}^{[1]}$.
In [24], we proposed to process directly the orientation matrix $\mathbf{U}$ with a specific *orthogonal matrix-preserving* PDE flow, that anisotropically regularized the field :

$$\frac{\partial \mathbf{U}}{\partial t} = -\mathbf{L} + \mathbf{U}\, \mathbf{L}^{\mathrm{T}}\, \mathbf{U}$$

where $\mathbf{L}$ is the matrix corresponding to the *unconstrained regularization term.*

- The orientation swapping problem : However, when dealing with diffusion tensors, one has to take care of the non-uniqueness of the spectral decomposition $\mathbf{T} = \sum_{k=1}^{n} \lambda_k\ \mathbf{u}^{[k]}\ \mathbf{u}^{[k]^T}$. Flipping one eigenvector direction while keeping its orientation (i.e considering $-\mathbf{u}^{[l]}$ instead of $\mathbf{u}^{[l]}$) gives the same tensor $\mathbf{T}$. It means that a constant tensor field may be decomposed into *highly discontinuous* orientation fields $\mathbf{U}$, disturbing the anisotropic regularization process with false discontinuity detections.
To overcome this problem, authors of [11, 24] proposed a *local eigenvector alignment process* that is done before applying the PDE on each tensor of the field $\mathbf{T}$. However, this is a very time-consuming process which dramatically slows down the algorithms.

3.3 Isospectral flow and orientation regularization

An alternative method exists, avoiding any eigenvector realignment problems. The idea lies on the use of an *isospectral flow*, that regularizes the tensor field *while preserving the eigenvalues of the considered tensors.* As a result, only tensor orientations are regularized. As we measure directly the tensor field variations from the gradients of the matrix coefficients, no false discontinuities are considered. The general form of an isospectral matrix flow is (see [9, 10]) :

$$\frac{\partial \mathbf{T}}{\partial t} = [\mathbf{T}, [\mathbf{T}, -(\mathbf{G} + \mathbf{G}^T)]] \quad \text{with} \quad [\mathbf{A}, \mathbf{X}] = \mathbf{AX} - \mathbf{XA} \tag{9}$$

Here, we choose the term $\mathbf{G}$ to correspond to the unconstrained form of the desired regularization process. It can be freely chosen. For instance, we used :

$$\mathbf{G} = (G_{i,j}) \quad \text{with} \quad G_{i,j} = \text{div}\left(\frac{\phi'(\|\nabla \mathbf{T}\|)}{\|\nabla \mathbf{T}\|} \nabla T_{i,j}\right)$$

where $\phi(s) = \sqrt{1+s^2}$ is a classical ϕ-function leading to discontinuity-preserving regularization [8]. Note that other regularization terms $\mathbf{G}$ may be suitable, as those proposed in [13, 20, 23, 25, 28], since the the Eq.(9) is a very general formalism to work on diffusion tensor orientations.
Like the estimation method, a specific numerical scheme based on matrix exponentials can be used to implement the isospectral PDE flow (9), avoiding any problems of numerical reprojections (see [9] for details) :

$$\mathbf{T}_{(t+dt)} = \mathbf{A}^T \mathbf{T}_{(t)} \mathbf{A} \quad \text{with} \quad \mathbf{A} = \exp\left(-dt[\mathbf{G} + \mathbf{G}^T, \mathbf{T}_{(t)}]\right)$$

This equation allows to speed up the process, since no eigenvector alignment is no more necessary. Moreover, the genericity of this approach allows to combine precise and adapted regularization terms with the advantage of the separate regularization of tensor orientations and diffusivities. The exponential maps-based scheme is numerically computed using *Padé approximations* [12] for matrix exponentials, while the unconstrained regularization term $\mathbf{G}$ is discretized with classical finite differences schemes.

4 Application to real DT-MRI datasets

We applied our proposed isospectral-based regularization algorithm in order to improve the fiber tracking on a real DT-MRI dataset (consisting in 121 images $128 \times 128 \times 56$, courtesy of CEA-SHFJ/Orsay-France). We first estimated the diffusion tensor field from the raw images, using our robust tensor estimation method eq.(5). Then, we regularized this obtained volume of tensors with our proposed spectral methods (eq.(8) and eq.(9)) (illustration on Fig.4).

Conclusion & Perspectives

We proposed original PDE-based alternatives to classical algorithms used to solve two crucial problems encountered in DT-MRI imaging. Our estimation and regularization algorithms ensures the positive-definite constraint of the tensors, thanks to specific constrained variational flows and corresponding numerical schemes based on the use of exponential maps. It leads then to fast and numerically stable algorithms. Finally, we illustrate these algorithms with fiber tractography in the white matter of the brain. As a perspective, we are working on similar constrained variational methods for more coherent fiber tracking, as proposed in [4, 6, 16, 17, 19, 27].

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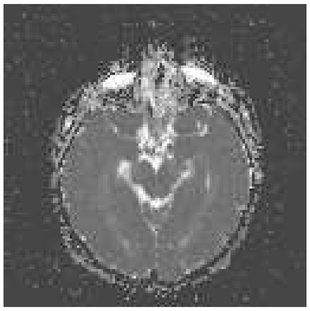
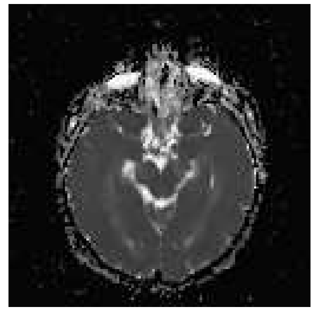
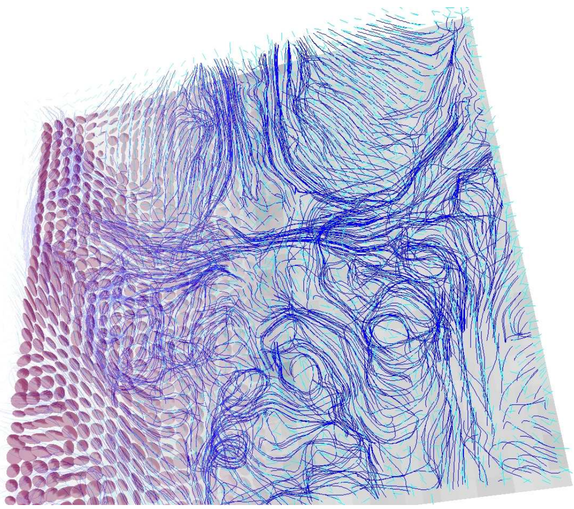


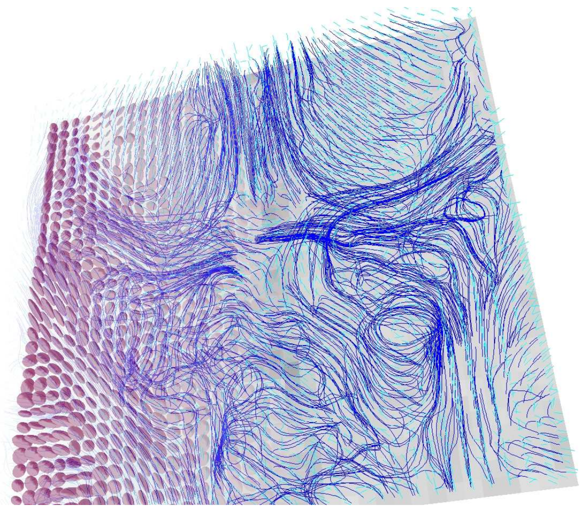
(a) Eigenvalues of an original DT-MRI volume



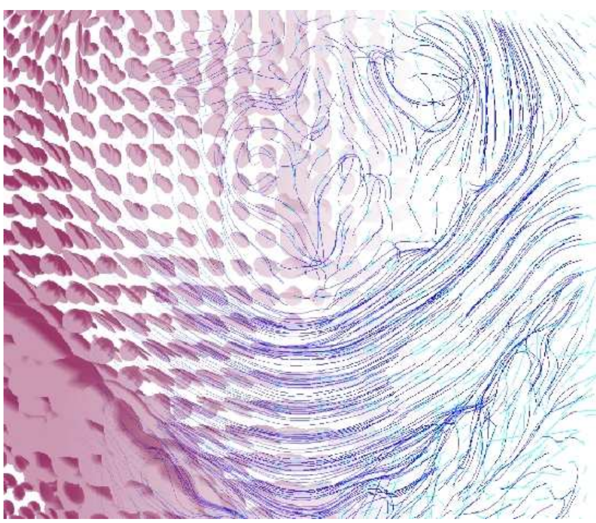
(b) Regularized eigenvalues with eq.(8)



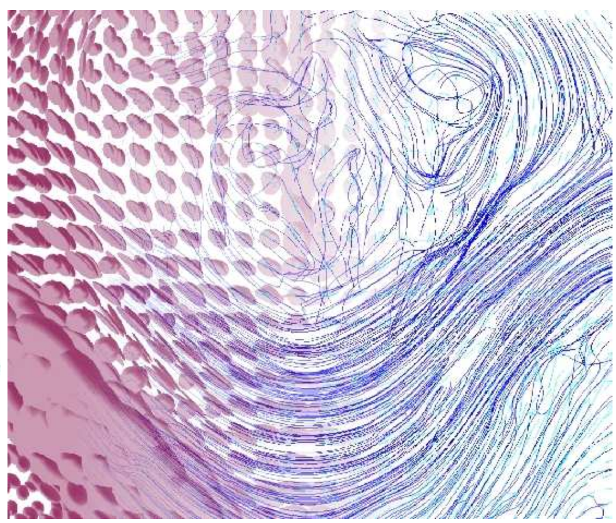
(c) Tensors/Fibers from the original data $\mathbf{T}$.



(d) Tensors/Fibers from the regularized data $\mathbf{T}_{\text{regul}}$.



(c) Part of the Corpus-callosum (Original)



(d) Part of the Corpus-callosum (Regularized)

Fig. 4. DT-MRI Regularization, using constrained spectral methods (eq.(8) and eq.(9)).