

A Bloch Torrey Equation for Diffusion in a Deforming Media

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Diffusion Process

Introduction to the Diffusion

Diffusion Equation

Illustrations of the Diffusion Process

MRI

Introduction

Static Case

Dynamic Case

Change of Coordinates

Curvilinear Coordinates

Prolate Spheroidal Coordinates

Numerical Solution

Implicit Method

Numerical Solution for the Bloch-Torrey Equation

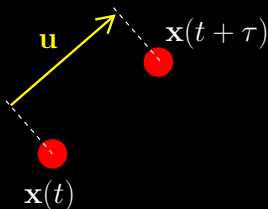
Diffusion Process

- ▶ Link Between **Microscopical** and **Macroscopical** Behavior.
- ▶ Expressed with the **Diffusion Coefficient**
 - ▶ Scalar Case:

$$6\tau D = [x(t + \tau) - x(t)]^2$$

- ▶ Vectorial Case:

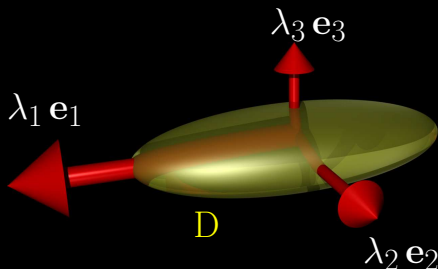
$$\begin{cases} 6\tau D = \mathbf{u}\mathbf{u}^T \\ \mathbf{u} = \mathbf{x}(t + \tau) - \mathbf{x}(t) \end{cases}$$



The Diffusion Tensor

- ▶ D is a **Symmetric Definite Positive** matrix by definition.

$$D = \sum_{i=1}^3 \lambda^i \mathbf{e}_i \mathbf{e}_i^T = \mathbf{R} \mathbf{\Lambda} \mathbf{R}^T$$



The Diffusion Equation

- ▶ For a scalar ϕ

$$\frac{\partial \phi}{\partial t} = \nabla \cdot \underbrace{(\mathbf{D} \nabla \phi)}_{\text{flux density}}$$

- ▶ For a vector $\phi = \phi^i \mathbf{e}_i$

$$\frac{\partial \phi^i}{\partial t} = \nabla \cdot (\mathbf{D} \nabla \phi^i)$$

- ▶ General Solution (\mathbf{D} independant of t with boundary conditions sent to infinity.)

$$\phi(\mathbf{x}, t) = \frac{1}{\sqrt{|\mathbf{D}|} (4\pi t)^{\frac{N}{2}}} e^{-\frac{\mathbf{x}^T \mathbf{D}^{-1} \mathbf{x}}{4t}} * \phi(\mathbf{x}, 0)$$

Illustration of the Diffusion Process

Exemple of the Action of the **Orientation** of the Diffusion Tensor:

1. Original Distribution
2. Filtered Distribution
3. Main Orientation of the Tensors

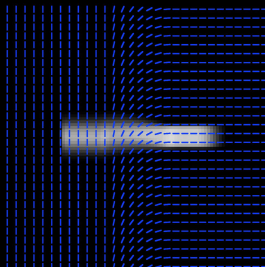


Illustration of the Diffusion Process (II)

Exemple of the Action of the **Inhomogeneous** Diffusion Phenomena Applied to the Filtering.

1. Original
2. Noisy
3. Homogeneous Gaussian Filtering
4. Inhomogeneous Diffusion



Bloch Equation

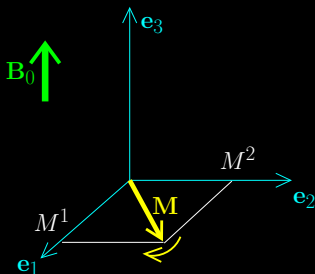
- ▶ ^1H atoms abundant in the water possess a nuclear angular momentum: the **Spin**.
- ▶ The orientation of the Spin is given by **M**.
- ▶ Under a Magnetic Field **B**, the momentum rotates around **B** at the pulsation $\gamma\|\mathbf{B}\|$:

$$\mathbf{M}_{,t} = \mathbf{M} \times \gamma \mathbf{B}$$

Bloch Equation (II)

- ▶ In order to acquire the momentum \mathbf{M} , a large Magnetic Field \mathbf{B}_0 is applied along the axis $z : \mathbf{e}_3$, and \mathbf{M} is flipped in the (x, y) plane by a special field.

$$\begin{cases} \mathbf{M}_{,t} = \mathbf{M} \times \gamma \mathbf{B} - \frac{M^1 \mathbf{e}_1 + M^2 \mathbf{e}_2}{T_2} - \frac{M^3 - M_0^3}{T_1} \mathbf{e}_3 \\ \mathbf{M}(\mathbf{x}, 0) = \mathbf{M}_0 \end{cases}$$



Bloch-Torrey Equation

The Diffusive term $\nabla \cdot (D \nabla \mathbf{M})$ is added:

$$\mathbf{M}_{,t} = \mathbf{M} \times \gamma \mathbf{B} - \frac{M^1 \mathbf{e}_1 + M^2 \mathbf{e}_2}{T_2} - \frac{M^3 - M_0^3}{T_1} \mathbf{e}_3 + \nabla \cdot (D \nabla \mathbf{M})$$

Where $\nabla \cdot (D \nabla \mathbf{M})$ has to be understood componentwise.

Attenuation Expression

It is first supposed that

- ▶ D does not depend on t , then for every position $D = \text{const.}$
- ▶ The diffusion seen by each molecule is constant along its displacement.

Attenuation Expression

- ▶ Only the (x, y) Components are Taken in Account:

$$\underline{M} = M^1 + i M^2$$

- ▶ The Magnetization Vector is Expressed as:

$$\underline{M}(\mathbf{x}, t) = A_{\mathbf{x}}(t) e^{-\alpha(t)} e^{i\varphi(\mathbf{x}, t)}$$

- ▶ The matrix B is defined:

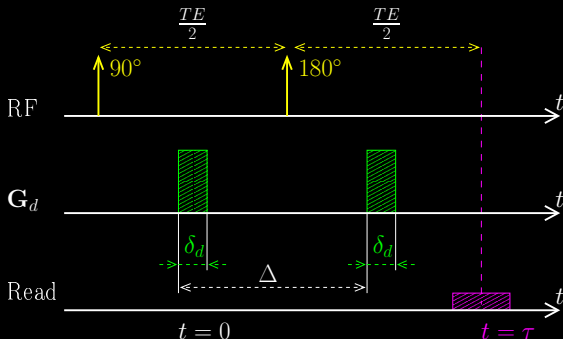
$$\begin{cases} \mathbf{B}(\mathbf{x}, t) = (\nabla\varphi) (\nabla\varphi)^T \\ \varphi = \gamma \int_0^t \mathbf{x} \cdot \mathbf{G}(t') dt' \quad !!! \end{cases}$$

- ▶ The Attenuation $A_{\mathbf{x}}$ is given by:

$$\ln \left(\frac{A_{\mathbf{x}}(t)}{A_{\mathbf{x}}(0)} \right) = -\text{tr} \left[\left(\int_0^t \mathbf{B}(\mathbf{x}, t') dt' \right) \mathbf{D} \right]$$

Special Pulse Sequence

$$\begin{cases} \ln \left(\frac{A_x(t)}{A_x(0)} \right) = -\Delta \mathbf{k}^T \mathbf{D} \mathbf{k} \\ \mathbf{k} = \gamma \delta \mathbf{G}_d \end{cases}$$



Deformed Referential

- ▶ The deformation is characterized by the tensorial **Deformation Gradient**:

$$\mathbf{F} = \frac{\partial \xi^i}{\partial X^j}$$

- ▶ And follow the relation:

$$d\xi = \mathbf{F} d\mathbf{X}$$

Expression of the gradient of phase

- ▶ The spatial phase variation has to be expressed in the fixed referential where the phase is:

$$\varphi(\boldsymbol{\xi}, t) = \gamma \int_0^t \mathbf{X}(\boldsymbol{\xi}, t') \cdot \mathbf{G}(t') dt'$$

- ▶ It is assumed a smooth deformation:

$$\nabla^T \varphi(\boldsymbol{\xi}, t) d\boldsymbol{\xi} = \nabla^T \varphi(\mathbf{X}, t) d\mathbf{X}$$

- ▶ Using the deformation Gradient \mathbf{F} :

$$\nabla \varphi(\boldsymbol{\xi}, t) = \mathbf{F}^{-T}(\mathbf{X}, t) \nabla \varphi(\mathbf{X}, t) d\mathbf{X}$$

Expression of the Diffusion tensor

The component of the tensor depends on the basis:

- ▶ The tensor expressed in the original referential: \bar{D}
- ▶ The tensor expressed in the deformed referential: D
- ▶ They are linked by the relation:

$$D_i^j = \frac{\partial \xi^i}{\partial X^k} \frac{\partial X^l}{\partial \xi^j} \bar{D}_l^k$$

$$\Rightarrow D = F \bar{D} F^{-1}$$

Expression of the Attenuation

- ▶ The Attenuation is Expressed with the Components of the Initial Referential:

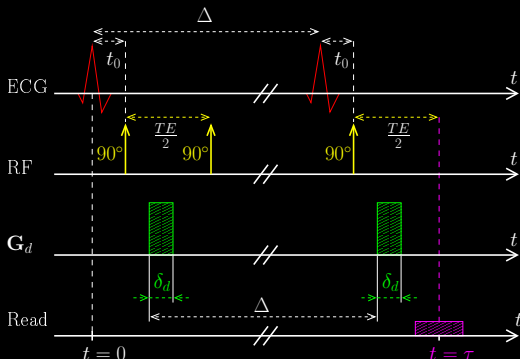
$$\ln \left(\frac{A_{\mathbf{x}}(t)}{A_{\mathbf{x}}(0)} \right) = \int_0^t (\nabla \varphi)^T \bar{\mathbf{D}} \mathbf{F}^{-2} \nabla \varphi dt'$$

- ▶ The **Right Stretch tensor** is introduced such that:
 $\mathbf{F}^T \mathbf{F} = \mathbf{U}^2$

$$\ln \left(\frac{A_{\mathbf{x}}}{A_{\mathbf{x}}} \right) = \int_0^t (\nabla \varphi)^T \bar{\mathbf{D}} \mathbf{U}^{-2} \nabla \varphi dt'$$

Aquisition Sequence

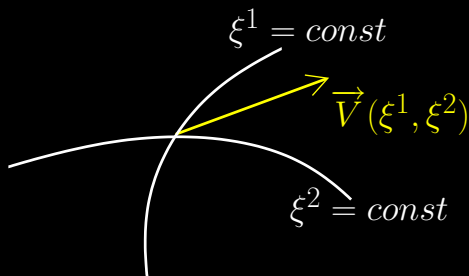
$$\begin{cases} \ln \left(\frac{A_{\mathbf{x}}(\tau)}{A_{\mathbf{x}}(0)} \right) = -\Delta \mathbf{k}^T \mathbf{D}_{\text{obs}} \mathbf{k} \\ \mathbf{D}_{\text{obs}} = \frac{1}{\Delta} \int_0^{\Delta} \overline{\mathbf{D}} U^{-2} dt \end{cases}$$



Use of the Curvilinear Coordinates

- ▶ A change of coordinates:

$$(\xi^1, \xi^2, \xi^3) = \phi(x^1, x^2, x^3)$$



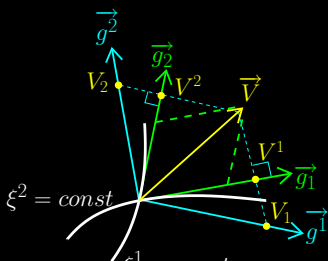
Curvilinear Basis

- ▶ A covariant basis \mathbf{g}_i such that $\mathbf{x} = x^i \mathbf{e}_i = \xi^i \mathbf{g}_i$:

$$\mathbf{g}_i = \frac{\partial \mathbf{x}^j}{\partial \xi^i} \mathbf{e}_j$$

- ▶ A contravariant basis \mathbf{g}^i :

$$\mathbf{g}^i = \frac{\partial \xi^i}{\partial \mathbf{x}^j} \mathbf{e}^j$$



Parameters of the Curvilinear Coordinates

- ▶ The Metric tensor:

$$g_{ij} = \mathbf{g}_i \cdot \mathbf{g}_j$$

- ▶ The ∇ operator given by:

$$\nabla = \mathbf{g}^i \frac{\partial}{\partial \xi^i}$$

- ▶ The Christoffel symbols of second kind Γ :

$$\left\{ \begin{array}{l} \mathbf{g}_{i,j} = \Gamma_{ij}^k \mathbf{g}_k \\ \Gamma_{jk}^i = \frac{\partial^2 x^l}{\partial \xi^j \partial \xi^k} \frac{\partial \xi^i}{\partial x^l} \end{array} \right.$$

Expression of the Bloch-Torrey Equation

- ▶ We use:

$$\mathbf{M}(\boldsymbol{\xi}, t) = M^i(\boldsymbol{\xi}, t) \mathbf{e}_i$$

- ▶ In the Cartesian case the Equation is:

$$\mathbf{M}_{,t} = \mathbf{M} \times \gamma \mathbf{B} - \frac{M^1 \mathbf{e}_1 + M^2 \mathbf{e}_2}{T_2} - \frac{M^3 - M_0^3}{T_1} \mathbf{e}_3 + \nabla \cdot (\mathbf{D} \nabla \mathbf{M})$$

- ▶ Only the diffusion $\nabla \cdot (\mathbf{D} \nabla M^i)$ term is modified:

Expression of the Diffusion in Curvilinear Coordinates

- ▶ The first term:

$$D \nabla M^i = D_j^k M_{,k}^i \mathbf{g}^j$$

- ▶ The diffusion term:

$$\nabla \cdot (D \nabla M^i) = \left[\left(D_k^l M_{,l}^i \right)_{,j} - \Gamma_{kj}^m D_m^l M_{,l}^i \right] \mathbf{g}^{jk}$$

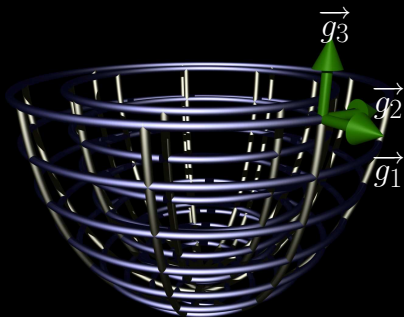
- ▶ The complete equation:

$$\mathbf{M}_{,t} = \mathbf{M} \times \gamma \mathbf{B} - \frac{M^1 \mathbf{e}_1 + M^2 \mathbf{e}_2}{T_2} - \frac{M^3 - M_0^3}{T_1} \mathbf{e}_3 + \left[\left(D_j^k \mathbf{M}_{,k} \right)_{,i} - \Gamma_{ji}^l D_l^k \mathbf{M}_{,k} \right] \mathbf{g}^{ij}$$

Definition of the Coordinates

- Change of variable:

$$\begin{cases} x^1 &= C \sinh(\xi^1) \sin(\xi^2) \cos(\xi^3) \\ x^2 &= C \sinh(\xi^1) \sin(\xi^2) \sin(\xi^3) \\ x^3 &= C \cosh(\xi^1) \cos(\xi^2) \end{cases}$$



Basis

- ▶ Contravariant basis vector:

$$\mathbf{g}_1 = C \begin{pmatrix} \cosh(\xi^1) \sin(\xi^2) \cos(\xi^3) \\ \cosh(\xi^1) \sin(\xi^2) \sin(\xi^3) \\ \sinh(\xi^1) \cos(\xi^2) \end{pmatrix}$$

$$\mathbf{g}_2 = C \begin{pmatrix} \sinh(\xi^1) \cos(\xi^2) \cos(\xi^3) \\ \sinh(\xi^1) \cos(\xi^2) \sin(\xi^3) \\ -\cosh(\xi^1) \sin(\xi^2) \end{pmatrix}$$

$$\mathbf{g}_3 = C \begin{pmatrix} \sinh(\xi^1) \sin(\xi^2) \sin(\xi^3) \\ -\sinh(\xi^1) \sin(\xi^2) \cos(\xi^3) \\ 0 \end{pmatrix}$$

Metric Tensor

- ▶ The Prolate basis is orthogonale.
- ▶ The metric tensor is diagonale:

$$[\mathbf{g}_{ij}] = C^2 \begin{pmatrix} \sinh^2(\xi^1) + \sinh^2(\xi^2) & 0 & 0 \\ 0 & \sinh^2(\xi^1) + \sinh^2(\xi^2) & 0 \\ 0 & 0 & \sinh(\xi^1) \sinh(\xi^2) \end{pmatrix}$$

- ▶ The element of volume is:

$$dx dy dz = C^3 \sinh(\xi^1) \sin(\xi^2) (\sinh^2(\xi^1) + \sinh^2(\xi^2)) d\xi^1 d\xi^2 d\xi^3$$

Christoffel Symbols

$$[\Gamma^1_{ij}] = \begin{pmatrix} \frac{\cosh(\xi^1) \sinh(\xi^1)}{\sinh^2(\xi^1) + \sin^2(\xi^2)} & \frac{\cos(\xi^2) \sinh(\xi^2)}{\sinh^2(\xi^1) + \sin^2(\xi^2)} & 0 \\ \frac{\cos(\xi^2) \sin(\xi^2)}{\sinh^2(\xi^1) + \sin^2(\xi^2)} & -\frac{\cosh(\xi^1) \sinh(\xi^1)}{\sinh^2(\xi^1) + \sin^2(\xi^2)} & 0 \\ 0 & 0 & -\frac{\sinh(\xi^1) \cosh(\xi^1) \sin^2(\xi^2)}{\sinh^2(\xi^1) + \sin^2(\xi^2)} \end{pmatrix}$$

$$[\Gamma^2_{ij}] = \begin{pmatrix} -\frac{\cos(\xi^2) \sin(\xi^2)}{\sinh^2(\xi^1) + \sin^2(\xi^2)} & \frac{\cosh(\xi^1) \sinh(\xi^1)}{\sinh^2(\xi^1) + \sin^2(\xi^2)} & 0 \\ \frac{\cosh(\xi^1) \sinh(\xi^1)}{\sinh^2(\xi^1) + \sin^2(\xi^2)} & \frac{\cos(\xi^2) \sin(\xi^2)}{\sinh^2(\xi^1) + \sin^2(\xi^2)} & 0 \\ 0 & 0 & -\frac{\sinh^2(\xi^1) \cos(\xi^2) \sin(\xi^2)}{\sinh^2(\xi^1) + \sin^2(\xi^2)} \end{pmatrix}$$

$$[\Gamma^3_{ij}] = \begin{pmatrix} 0 & 0 & \operatorname{cotanh}(\xi^1) \\ 0 & 0 & \operatorname{cotan}(\xi^2) \\ \operatorname{cotanh}(\xi^1) & \operatorname{cotan}(\xi^2) & 0 \end{pmatrix}$$

Expression of the Equation

- ▶ The equation is simplified by the use of an orthogonal coordinate system:

$$\mathbf{M}_{,t} = \mathbf{M} \times \gamma \mathbf{B} - \frac{M^1 \mathbf{e}_1 + M^2 \mathbf{e}_2}{T_2} - \frac{M^3 - M_0^3}{T_1} \mathbf{e}_3 +$$

$$+ \sum_{i=1}^3 \left(g^{ii} \left[\sum_{j=1}^3 \left(D_{i,j}^j \mathbf{M}_{,ji} + D_{i,i}^j \mathbf{M}_{,j} - \Gamma_{ii}^j \sum_{k=1}^3 \left(D_j^k \mathbf{M}_{,k} \right) \right) \right] \right)$$

- ▶ Possibility of animating it: For instance, an easy dilatation

$$\xi'^1 = a(t) \xi^1$$

Finite Differences methods in one dimension

- ▶ The central difference operator:

$$\mathcal{D}^1 M = M(x + \Delta x) - M(x - \Delta x)$$

- ▶ Second order accurate:

$$\left| \frac{\mathcal{D}^1 M}{2\Delta x} - \frac{\partial M}{\partial x} \right| \leq A |\Delta x|^2$$

- ▶ The second spatial derivative

$$\mathcal{D}^{11} M = M(x + \Delta x) - 2M(x) + M(x - \Delta x)$$

- ▶ Second order accurate too

$$\left| \frac{\mathcal{D}^{11} M}{(\Delta x)^2} - \frac{\partial^2 M}{\partial x^2} \right| = \mathcal{O}(|\Delta x|^2)$$

Vector and matrix notation

- ▶ The function is discretized on a spatial grid of N intervals of size Δx .
- ▶ The function is stored as a vector \mathbf{u} such that:

$$M(k\Delta x) = u[k]$$

- ▶ The difference operator acting on the vector is the matrix:

$$[\mathcal{D}^1]_{i,j} = \begin{cases} 1 & \text{if } i = j - 1 \\ -1 & \text{if } i = j + 1 \\ 0 & \text{otherwise} \end{cases}$$

$$[\mathcal{D}^{11}]_{i,j} = \begin{cases} 1 & \text{if } i = j - 1 \\ -2 & \text{if } i = j \\ 1 & \text{if } i = j + 1 \\ 0 & \text{otherwise} \end{cases}$$

Solution of the Diffusion Equation

- ▶ The one dimensional diffusion equation is:

$$\frac{\partial M}{\partial t} = D \Delta M$$

- ▶ Using the notation $\mathbf{u}(t) = \mathbf{u}$ and $\mathbf{u}(t + \Delta t) = \mathbf{u}^+$. The new equation can be:

$$\frac{\mathbf{u}^+ - \mathbf{u}}{\Delta t} = \frac{D}{(\Delta x)^2} \mathcal{D}^{11} \mathbf{u} \quad \text{or} \quad \frac{\mathbf{u}^+ - \mathbf{u}}{\Delta t} = \frac{D}{(\Delta x)^2} \mathcal{D}^{11} \mathbf{u}^+$$

Explicit and Implicit method

- ▶ Two algorithms:
 - ▶ Explicit Method (easy to implement):

$$\mathbf{u}^+ = \left(\mathbf{I}_N + D \frac{\Delta t}{(\Delta x)^2} \mathcal{D}^{11} \right) \mathbf{u}$$

- ▶ Implicit Method (linear system to solve):

$$\left(\mathbf{I}_N - D \frac{\Delta t}{(\Delta x)^2} \mathcal{D}^{11} \right) \mathbf{u}^+ = \mathbf{u}$$

Crank-Nichols Scheme

- ▶ A stable second order accurate method can also be used and states that:

$$\frac{1}{\Delta t} \mathcal{D}^t \mathbf{u} = \frac{D}{(\Delta x)^2} \mathcal{D}^{11} \frac{\mathbf{u}^+ + \mathbf{u}}{2}$$

Operator in three dimensions

- ▶ The operators are defined in three dimensions:

$$\mathcal{D}^i \mathbf{M} = \mathbf{M}(\xi^i + \Delta\xi^i) - \mathbf{M}(\xi^i - \Delta\xi^i)$$

$$\mathcal{D}^{ii} \mathbf{M} = \mathbf{M}(\xi^i + \Delta\xi^i) - 2\mathbf{M}(\xi^i) + \mathbf{M}(\xi^i - \Delta\xi^i)$$

$$\begin{aligned} \mathcal{D}^{ij} \mathbf{M} = & +\mathbf{M}(\xi^i + \Delta\xi^i, \xi^j + \Delta\xi^j) \\ & -\mathbf{M}(\xi^i - \Delta\xi^i, \xi^j + \Delta\xi^j) \\ & -\mathbf{M}(\xi^i + \Delta\xi^i, \xi^j - \Delta\xi^j) \\ & +\mathbf{M}(\xi^i - \Delta\xi^i, \xi^j - \Delta\xi^j) \end{aligned}$$

Vector Notation

- ▶ The spatial grid of size $N_1 \times N_2 \times N_3$ is created and each voxel has a volume $\Delta\xi^1 \times \Delta\xi^2 \times \Delta\xi^3$.
- ▶ The discrete function \mathbf{M} is stored in a large vector \mathbf{u} such that:

$$M^i(k_1\Delta\xi^1, k_2\Delta\xi^2, k_3\Delta\xi^3) = u[i + 3(k_1 + N_1(k_2 + N_2 k_3))]$$

Matrix Notation

- ▶ The derivative matrix are very large matrix of size $(3 N_1 N_2 N_3)^2$
- ▶ For each line l and column J the associated parameters are $(i^l, k_1^l, k_2^l, k_3^l)$ for the lines and $(i^c, k_1^c, k_2^c, k_3^c)$ for the columns.
- ▶ An example of a derivative matrix is:

$$[\mathcal{D}^{12}]_{l,J} = \begin{cases} 1 & \text{if } \begin{cases} (i^l, k_1^l, k_2^l, k_3^l) = (i^c, k_1^c + 1, k_2^c + 1, k_3^c) \\ (i^l, k_1^l, k_2^l, k_3^l) = (i^c, k_1^c - 1, k_2^c - 1, k_3^c) \end{cases} \\ -1 & \text{if } \begin{cases} (i^l, k_1^l, k_2^l, k_3^l) = (i^c, k_1^c + 1, k_2^c - 1, k_3^c) \\ (i^l, k_1^l, k_2^l, k_3^l) = (i^c, k_1^c - 1, k_2^c + 1, k_3^c) \end{cases} \\ 0 & \text{otherwise} \end{cases}$$

Numerical Equation

- ▶ $\mathbf{M} \times \gamma \mathbf{B}$ is also expressed in matrix form $\mathbf{G}\mathbf{u}$.
- ▶ The projections onto the \mathbf{e}_m axis are also defined by P^m .
- ▶ Calling \mathbf{u}_0^z the corresponding vector for $P^3 \mathbf{u}(t=0)$, the Bloch-Torrey Equation is:

$$\mathcal{D}^t \mathbf{u} = \left(\mathbf{G} - \frac{P^1 + P^2}{T_2} + \frac{P^3}{T_1} + \left[D_j^k \cdot {}_i \mathbf{I} + D_j^k \mathcal{D}^i - \Gamma_{ji}^l D_l^k \mathcal{D}^k \right] \right) \mathbf{u} - \frac{\mathbf{u}_0^z}{T_1}$$

- ▶ Written in the form:

$$\mathcal{D}^t \mathbf{u} = \mathbf{S}\mathbf{u} + \mathbf{s}$$

Crank-Nicholson Method

- ▶ The Crank-Nicholson method is used:

$$\frac{\mathbf{u}^+ - \mathbf{u}}{\Delta t} = \mathcal{S} \frac{\mathbf{u}^+ + \mathbf{u}}{2} + \mathbf{s}$$

- ▶ The equation is reorganized:

$$\left(\mathbf{I} - \Delta t \frac{\mathcal{S}}{2} \right) \mathbf{u}^+ = \left(\mathbf{I} + \Delta t \frac{\mathcal{S}}{2} \right) \mathbf{u} + \mathbf{s}$$

- ▶ Which is a simple linear system:

$$\mathcal{A} \mathbf{u}^+ = \mathbf{b}$$

Algorithm

- ▶ build matrices $\mathcal{D}^i, \mathcal{D}^{ij}, P^i$ and vector \mathbf{u}_0^z
- ▶ for all t
 - ▶ for all ξ
 - ▶ Build matrix $G (= \mathbf{M} \times \gamma (\mathbf{B} + \mathbf{x} \cdot \mathbf{G}))$
 - ▶ Multiply each lines with the coefficients : D_j^k, Γ_{ji}^l
 - ▶ end
- ▶ Build matrix \mathcal{A} and vector \mathbf{b}
- ▶ Solve for $\mathbf{u}^+ : \mathcal{A} \mathbf{u}^+ = \mathbf{b}$
- ▶ end

Limitations and Future Work

- ▶ Size of the linear system:

$$N \simeq N_1 \simeq N_2 \simeq N_3 \simeq 64 \Rightarrow \text{size} = (3N^3)^2 \simeq 62 \cdot 10^{10}$$

- ▶ Matrix \mathcal{A} is sparse but not tridiagonal \Rightarrow Time to invert the system.
 - ▶ Possibility of speeding-up by using the ADI (Alternative Direction Implicit) scheme ...