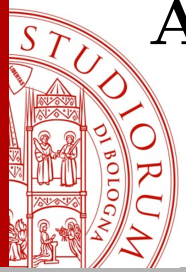

ModelFreeFFC and MUPen2D Software Tools

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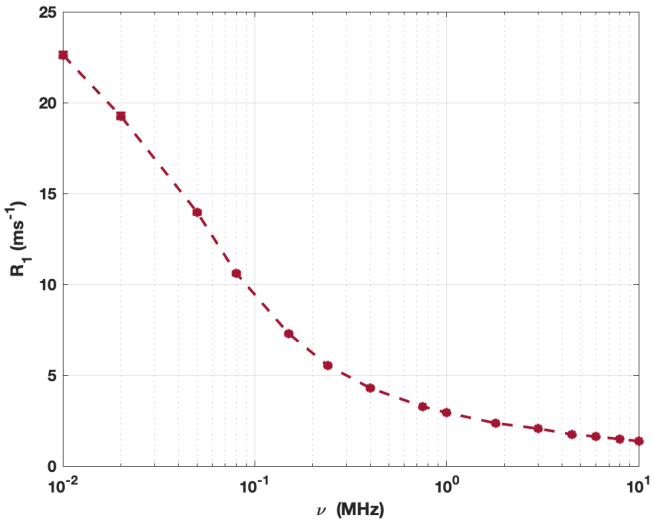
ModelFreeFFC

Fast Field Cycling (FFC) NMR Technique

Fast Field Cycling Nuclear Magnetic Resonance (FFC – NMR) is a non-destructive low-field magnetic resonance technique that allows to revealing information about molecular dynamics, and it measures the spin-lattice relaxation rate, $R_1 = \frac{1}{T_1}$, as a function of NMR frequency, ν ($\omega = 2\pi\nu$), over the kHz to MHz range.
This technique consists in rapidly changing the strength varying the intensity of the applied polarizing magnetic field, $\boldsymbol{B}_0$, causing the alteration of proton resonant frequency, and the measurement of R_1 as a function of Larmor angular frequency.



Relaxation rates can be represented as linear combinations of spectral density functions of the motion modulating the interactions.
However, complex spin dynamical interactions may occur such as the Quadrupole Relaxation Enhancement (QRE) due to their intramolecular magnetic dipolar coupling with quadrupole nuclei of arbitrary spins $S \geq 1$.
The presence of QRE is represented by local peaks of the R_1 profiles due to resonant phenomena, and its positions are strongly dependent on the physical and chemical nature of the sample.

FFC Mathematical Problem

$$R_1(\omega) = R_0 + R^{HH}(\omega) + R^{NH}(\omega) \tag{1}$$

- $R_1(\omega)$ is the acquired longitudinal relaxation rate.

[1] D.Kruk, et Al., *Dynamics of solid proteins by means of nuclear magnetic resonance relaxometry*, Biomolecules, 9 (11), 2019

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$$R^{HH}(\omega) = \int_0^\infty \left[\frac{\tau_c}{(1 + (\omega\tau_c)^2)} + \frac{4\tau_c}{(1 + 4(\omega\tau_c)^2)} \right] f(\tau_c)\, d\tau_c \tag{2}$$

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- $R^{NH}(\omega)$ describes the QRE[1] with unknown parameters $\boldsymbol{\psi} \in \mathbb{R}^6$.

$$R^{NH}(\omega) = C^{NH} \left[\left(\frac{1}{3} + \sin^2(\Theta)\cos^2(\Phi) \right) \left(\frac{\tau_Q}{1 + (\omega - \omega_-)^2 {\tau_Q}^2} + \frac{\tau_Q}{1 + (\omega + \omega_-)^2 {\tau_Q}^2} \right) + \right.$$

$$+ \left(\frac{1}{3} + \sin^2(\Theta)\sin^2(\Phi) \right) \left(\frac{\tau_Q}{1 + (\omega - \omega_+)^2 {\tau_Q}^2} + \frac{\tau_Q}{1 + (\omega + \omega_+)^2 {\tau_Q}^2} \right) + \tag{3}$$

$$\left. + \left(\frac{1}{3} + \cos^2(\Theta) \right) \left(\frac{\tau_Q}{1 + (\omega - (\omega_+ - \omega_-))^2 {\tau_Q}^2} + \frac{\tau_Q}{1 + (\omega + (\omega_+ - \omega_-))^2 {\tau_Q}^2} \right) \right]$$

[1] D.Kruk, et Al., *Dynamics of solid proteins by means of nuclear magnetic resonance relaxometry*, Biomolecules, 9 (11), 2019

Discrete Problem

$$\boldsymbol{y} = R_0 + \mathcal{F}_1(\boldsymbol{f}) + \mathcal{F}_2(\boldsymbol{\psi}) \tag{4}$$

where

- $\boldsymbol{\omega} \in \mathbb{R}^m$ represents the vector of the m Larmor angular velocity at which the NMRD profile is evaluated ($\omega = 2\pi\nu$, ν is in MHz).
- $\boldsymbol{y} \in \mathbb{R}^m$ represents the observation vector: $y_i = R_1(\omega_i)$, $i = 1, \ldots, m$.
- $\mathcal{F}_1(\boldsymbol{f}) : \mathbb{R}^n \to \mathbb{R}^m$ is linear and is obtained by discretizing R^{HH}:

$$\mathcal{F}_1(\boldsymbol{f}) \equiv \boldsymbol{K}\boldsymbol{f}, \quad \boldsymbol{K}_{i,j} = \frac{\tau_j}{\left(1 + (\omega_i \tau_j)^2\right)} + \frac{4\tau_j}{\left(1 + 4\,(\omega_i \tau_j)^2\right)}, \quad i = 1, \ldots, m \text{ and } j = 1, \ldots, n$$

Linear system of dimension $m \times n$ (usually $n > m$). τ_j are logarithmic uniformly distributed in the range $[10^{-3} - 10^{1}]$ μs.

- $\mathcal{F}_2(\boldsymbol{\psi}) : \mathbb{R}^6 \rightarrow \mathbb{R}^m$ is obtained by discretizing the quadrupolar component R^{NH}:

$$(\mathcal{F}_2(\boldsymbol{\psi}))_i = \psi_1 \left(\frac{1}{3} + \psi_2(1-\psi_3), \quad \frac{1}{3} + \psi_2\psi_3, \quad \frac{1}{3} + (1-\psi_2) \right) \cdot \begin{pmatrix} \frac{\psi_4}{1+(\omega_i-\psi_5)^2\psi_4^2} + \frac{\psi_4}{1+(\omega_i+\psi_5)^2\psi_4^2} \\ \frac{\psi_4}{1+(\omega_i-\psi_6)^2\psi_4^2} + \frac{\psi_4}{1+(\omega_i+\psi_6)^2\psi_4^2} \\ \frac{\psi_4}{1+(\omega_i-(\psi_6-\psi_5))^2\psi_4^2} + \frac{\psi_4}{1+(\omega_i+(\psi_6-\psi_5))^2\psi_4^2} \end{pmatrix}$$

- $\psi_1 \equiv C^{NH}$ represents the gyromagnetic ratios and the average interaction distance of the nuclei.
- $\psi_2 \equiv \sin^2(\Theta)$ and $\psi_3 \equiv \cos^2(\Phi)$ with Θ and Φ the two angles accounting for the orientation of the ${}^1H - {}^{14}N$ dipole-dipole axis with respect to the principal axis system of the electric field gradient at the position of ${}^{14}N$.
- $\psi_4 \equiv \tau_Q$ represents the correlation time for the ${}^1H - {}^{14}N$ quadrupolar interaction.
- $\psi_5 \equiv \omega_-$ and $\psi_6 \equiv \omega_+$ are the relevant characteristic angular frequencies.

Parameter Identification Problem

The parameter identification problem can be formulated as a *L_1-Regularized non-linear least squares problem*

$$\begin{aligned} \min_{\boldsymbol{f},\boldsymbol{\psi},R_0} \quad & \|\boldsymbol{y} - (\mathcal{F}_1(\boldsymbol{f}) + \mathcal{F}_2(\boldsymbol{\psi}) + R_0)\|_2^2 + \lambda\|\boldsymbol{f}\|_1 \\ \text{s.t.} \quad & \boldsymbol{f} \geq \mathbf{0}, \\ & \boldsymbol{\psi} \in \mathcal{B}_\psi, \\ & R_0 \geq 0 \end{aligned} \tag{5}$$

where the set $\mathcal{B}_\psi$ fixes the box constraints on ψ:

$$\mathcal{B}_\psi = \{\boldsymbol{\psi} \,:\, \psi_1 \in [C_\ell, C_u];\ \psi_2, \psi_3 \in [0,1];\ \psi_4 \in [\tau_\ell, \tau_n];\ \psi_5, \psi_6 \in [\omega_\ell, \omega_u]\}$$

and $\lambda > 0$ is the *regularization parameter*.

Problem Reformulation

By introducing two auxiliary variables

$$\boldsymbol{x}_1 \equiv (\boldsymbol{f}, R_0) \quad \text{and} \quad \boldsymbol{x}_2 = \boldsymbol{\psi}$$

the problem can be reformulated as

$$\begin{aligned} \min_{\boldsymbol{x}_1, \boldsymbol{x}_2} \quad & \|\boldsymbol{y} - \boldsymbol{K}_e \boldsymbol{x}_1 - \mathcal{F}_2(\boldsymbol{x_2})\|_2^2 + \lambda \|\boldsymbol{x}_1\|_1 + \eta \|\boldsymbol{x}_1\|_2^2 \\ \text{s.t.} \quad & \boldsymbol{x}_1 \in \boldsymbol{X}_1, \\ & \boldsymbol{x}_2 \in \boldsymbol{X}_2 \end{aligned} \tag{6}$$

where

- $\boldsymbol{X}_1 \equiv \boldsymbol{x}_1 \geq 0$
- $\boldsymbol{X}_2 \equiv \mathcal{B}_\psi$
- $\boldsymbol{K}_e = [\boldsymbol{K}\ 1] \in \mathbb{R}^{m \times (n+1)}$

The last term in the minimum problem, $\eta \|\boldsymbol{x}_1\|_2^2$ has been introduced to ensure that $\boldsymbol{K}_e^T \boldsymbol{K}_e + \eta \boldsymbol{I}$ is a positive definite matrix[2].

[2] $\eta = 10^{-10}$. Details and proofs in G. Landi, G.V. Spinelli, F. Zama, D.C. Martino, P. Conte, P.Lo Meo, and V. Bortolotti, *An Automatic L1-based regularization method for the analysis of FFC dispersion profiles with quadrupolar peaks*, Applied Mathematics and Computation, 2023.

Algorithm

Set $k = 0$, $\eta = 10^{-10}$, and choose a starting guess $\lambda^{(0)}$
Repeat

1. Determine $(\boldsymbol{x}_1^{(k)}, \boldsymbol{x}_2^{(k)})$ by solving

$$\begin{aligned} \arg \quad & \min \|\boldsymbol{y} - \boldsymbol{K}_e \boldsymbol{x}_1 - \mathcal{F}_2(\boldsymbol{x_2})\|_2^2 + \lambda \|\boldsymbol{x}_1\|_1 + \eta \|\boldsymbol{x}_1\|_2^2 \\ & \boldsymbol{x}_1 \in \boldsymbol{X}_1, \\ & \boldsymbol{x}_2 \in \boldsymbol{X}_2 \end{aligned} \tag{7}$$

   with the *constrained two-blocks non-linear Gauss Seidel* (GS) method[a].

2. Update the regularization parameter $\lambda^{(k+1)}$ using the balancing principle[b], such that

$$\lambda^{(k+1)} = \frac{\|\boldsymbol{y} - \boldsymbol{K}_e \boldsymbol{x}_1^{(k)} - \mathcal{F}_2(\boldsymbol{x}_2^{(k)})\|_2^2}{\|\boldsymbol{x}_1^{(k)}\|_1} \tag{8}$$

3. Compute $k = k + 1$

Until $|\lambda^{(k-1)} - \lambda^{(k)}| < \text{Tol}\, \lambda^{(k)}$

---

[a] L. Grippo, M. Sciandrone, *On the convergence of the block non-linear Gauss-Seidel method under convex constraints*. Operations research letters, 26(3), 2000

[b] K. Ito, B. Jin, and T. Takeuchi, *A Regularization Parameter for Nonsmooth Tikhonov Regularization*, SIAM Journal on Scientific Computing, vol. 33, no.3, 2011.

Gauss-Seidel Method

The constrained two-blocks non-linear Gauss-Seidel (GS) method is used for the solution of the L_1-regularized non-linear least squares problem (7).

2-Blocks GS method

1. Set $j = 0$ and choose a starting guess $(\boldsymbol{x}_1^{(0)}, \boldsymbol{x}_2^{(0)})$
2. **for** $j = 0, 1, \ldots$ **do**
3. Set $\boldsymbol{x}_1^{(j+1)} \in \arg\min_{\boldsymbol{z} \in \boldsymbol{X}_1} f(\boldsymbol{z}, \boldsymbol{x}_2^{(j)})$ — Truncated Newton interior-point method
4. Set $\boldsymbol{x}_2^{(j+1)} \in \arg\min_{\boldsymbol{z} \in \boldsymbol{X}_2} f(\boldsymbol{x}_1^{(j+1)}, \boldsymbol{z})$ — Newton Projection method
5. Set $\boldsymbol{x}^{(j+1)} = (\boldsymbol{x}_1^{(j+1)}, \boldsymbol{x}_2^{(j+1)})$
6. **end for**

Stopping criteria: $\dfrac{\left| f\left(\boldsymbol{x}_1^{(j+1)}, \boldsymbol{x}_2^{(j+1)}\right) - f\left(\boldsymbol{x}_1^{(j)}, \boldsymbol{x}_2^{(j)}\right) \right|}{f\left(\boldsymbol{x}_1^{(j+1)}, \boldsymbol{x}_2^{(j+1)}\right)} \leq \text{Tol or } j > K_{\max}$

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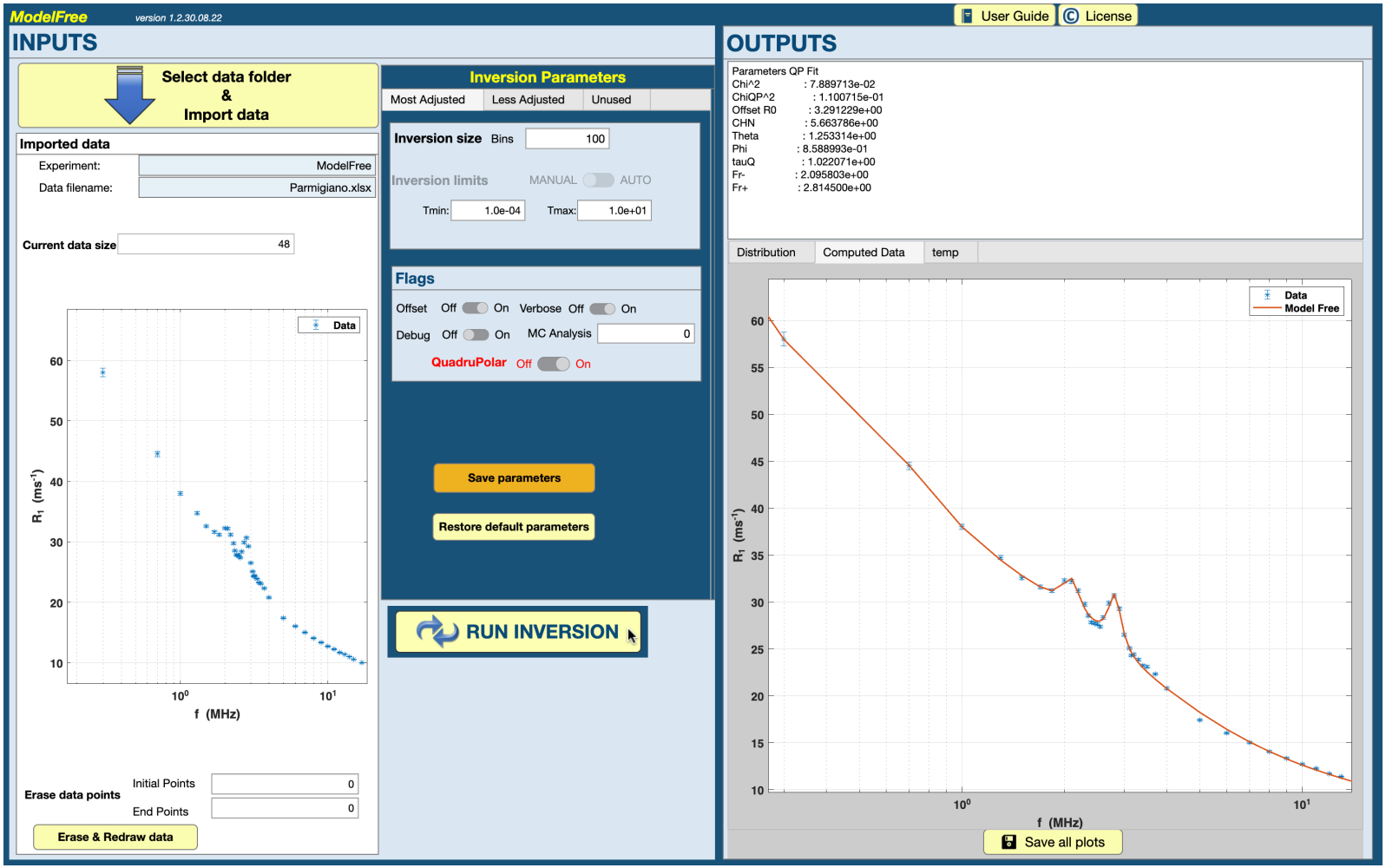
Mathematical properties

- ☐ The L_1-regularized non-linear least squares problem has solutions.
- ☐ The GS method is well defined, i.e., each sub-problem has solutions.
- ☐ The sequence $(\boldsymbol{x}_1^{(k)}, \boldsymbol{x}_2^{(k)})$ generated by the GS method converges to critical points.

Details and proofs in F. Zama et Al. *An Automatic L1-based regularization method for the analysis of FFC dispersion profiles with quadrupolar peaks*, 2022.

ModelFreeFFC Software[3]



[3] https://site.unibo.it/softwaredicam/en/modelfree

Data Folder

FileFlag.par

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Flags for experiment ModelFree
%
   FL_typeKernel         =3
   FL_InversionTimeLimits=1
   FL_Verbose            =1
   FL_Debug              =0
   FL_Amp_scale          =1
   FL_Scale_fact         =1
   FL_EraseCol           =0
   FL_EraseRow           =0
   FL_Offset             =1
   FL_Stat               =5
   FL_DispersionPars     =5
   FL_QPfitting          =1
END
```

FilePar.par

```
Inversion Parameters for experiment ModelFree

%[Linear L1Ls parameters]
   par.l1ls.tol          =1.0e-02
   par.l1ls.maxiter      =1.0e+03
   par.l1ls.duality      =1.0e-05
   par.l1ls.lambda       =1.0e-01
%
%[QuadruPolar L1Ls parameters]
   par.QP.lambda0        =1.0E-05
   par.QP.rel_tol        =1.0E-04
   par.QP.FrUp           =3.4
   par.QP.FrLo           =2.3
   par.QP.FrM0           =2.5
   par.QP.FrP0           =3.1
   par.QP.tauQ0          =4.8
   par.QP.CNH0           =11.5
   par.QP.CHNUpB         =100
   par.QP.tauQUpB        =100
   par.QP.GSMaxit        =500
   par.QP.GSTol          =1.0E-06
   par.QP.lambdaTol      =1.0E-02
   par.QP.PNwMaxit       =2000
   par.QP.PNwTol         =1.0E-06
   par.QP.LevMark        =1.0E-08
%
%[Solver parameters]
   par.Solver.maxiter    =1.0E+03
   par.Solver.tol        =1.0E-02
%
END
```

FileSetInput.par

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Filenames e parameters for inversion ModelFree
%
% [File Data]
   filenamedata          =NanoSpugna_secca.xlsx
% [Inversion Points]
   nbin                  =100
% [Inversion Time limits]
   T1min                 =1.0e-04
   T1max                 =1.0e+01
%
END
```
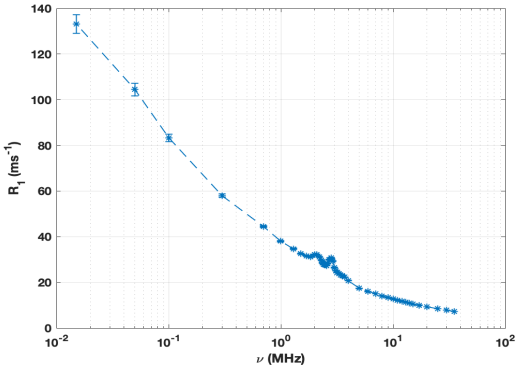
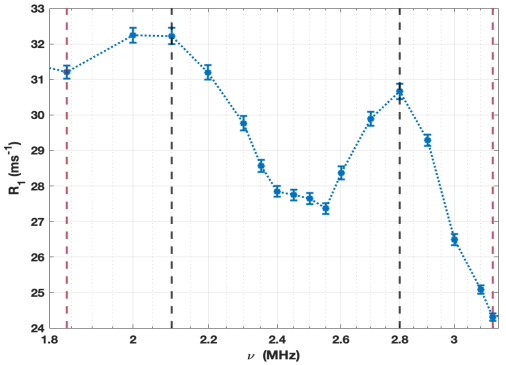

Data

	A	B	C	D	E	F
	35	7.0795	0.03349			
	30	8.157	0.04409			
	25	9.6784	0.05154			
	20	11.953	0.08924			
	17	13.412	0.08856			
	15	15.138	0.15934			
	14	16.439	0.16977			
	13	17.085	0.22678			
	12	18.808	0.28652			
0	11	19.837	0.32355			
1	10	21.085	0.21049			
2	9	24.277	0.46435			
3	8	26.894	0.40882			
4	7	31.158	0.51615			
5	6	34.657	0.56455			
6	5	41.762	0.51384			
7	4	56	0.5			
8	3.4	75.713	0.47828			
9	3.3	93.86	0.94234			
0	3.2	103.91	0.9007			
1	3.15	109.29	0.81266			
2	3.10	107.14	0.91925			
3	3.05	100.97	0.69793			
4	3.0	93.648	0.73492			
5	2.9	88.166	0.77939			
6	2.8	94.887	0.96211			
7	2.7	101.65	0.7832			
8	2.6	101.08	0.76389			
9	2.55	103.77	0.76851			
0	2.50	104.85	0.83886			
1	2.45	103.44	0.81158			
2	2.40	100.19	0.93085			
3	2.35	96.555	0.80397			
4	2.3	91.754	0.63763			

Results: Parmigiano-Reggiano cheese sample[4]

NMRD profile with $m = 48$ values with confidence intervals ranging from +0.35% to 3.07% of the value. Quadrupolar peaks at frequencies ($\nu_- = 2.1$ MHz, $R_{1\_} = 32.2\text{ms}^{-1}$), and ($\nu_+ = 2.8$ MHz, $R_{1+} = 30.7\text{ms}^{-1}$).





Initialization

$$\mathcal{B}_\psi = \{\boldsymbol{\psi} : \psi_1 \in [C_\ell, C_u];\ \psi_2, \psi_3 \in [0,1];\ \psi_4 \in [\tau_\ell, \tau_u];\ \psi_5, \psi_6 \in [\omega_\ell, \omega_u]\}.$$
$$C_\ell = 0, \quad C_u = 10^2, \quad \tau_\ell = 0, \quad \tau_u = 10^2, \quad \omega_\ell \approx 1.8(2\pi), \quad \omega_u \approx 3.2(2\pi).$$

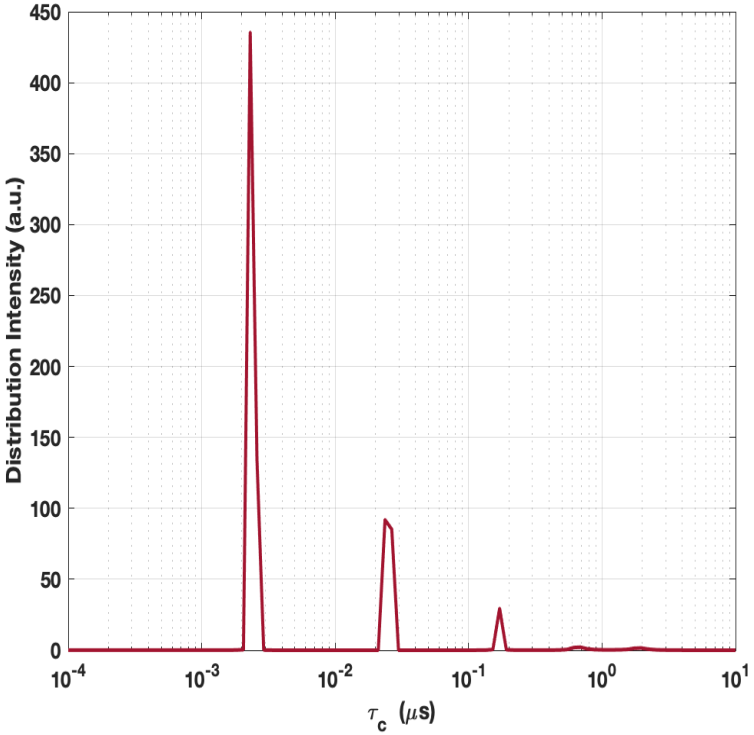
$$\boldsymbol{x}_1^{(0)} = (f^{(0)} = 1, R_0^{(0)} = 1).$$

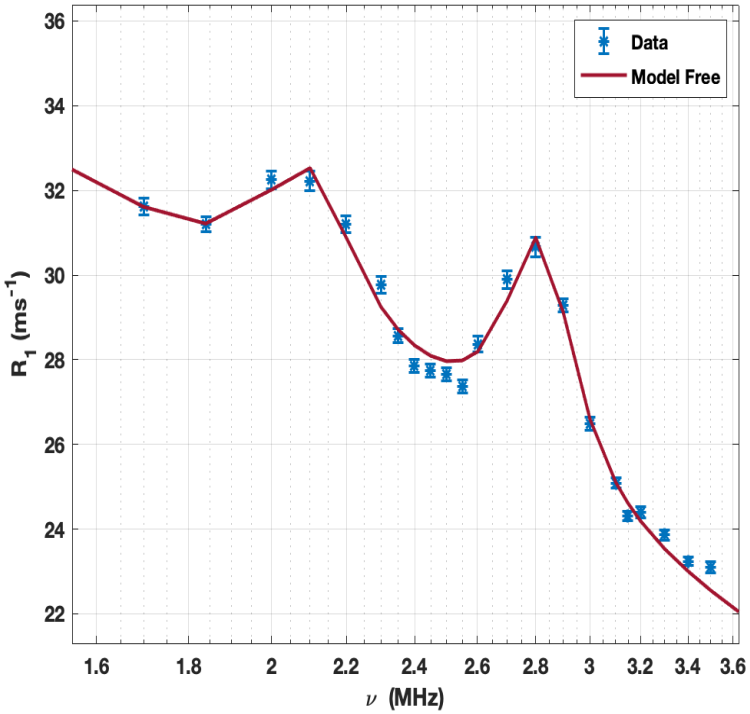
$$\lambda^{(0)} = 10^{-5}.$$

$$\boldsymbol{x}_2^{(0)} = \left\{ \boldsymbol{\psi}_1^{(0)} = \frac{2}{3}\left(\frac{\mu_0}{4\pi}\frac{\gamma_H \gamma_N \hbar}{r_{NH}^3}\right)^2 \approx 0.18\left[\frac{\mu s}{s^2}\right], \psi_2^{(0)} = \psi_3^{(0)} = 0.5, \psi_4^{(0)} = 1, \right.$$
$$\left. \psi_5^{(0)} = \omega_\ell + 0.25|\omega_u - \omega_\ell|, \psi_6^{(0)} = \omega_u - 0.25|\omega_u - \omega_\ell| \right\}.$$

[4] Data from P. Conte et Al., *Heuristic algorithm for the analysis of fast field cycling (FFC) NMR dispersion curves.* Analytical Chemistry, 93 (24), 2021.

Results



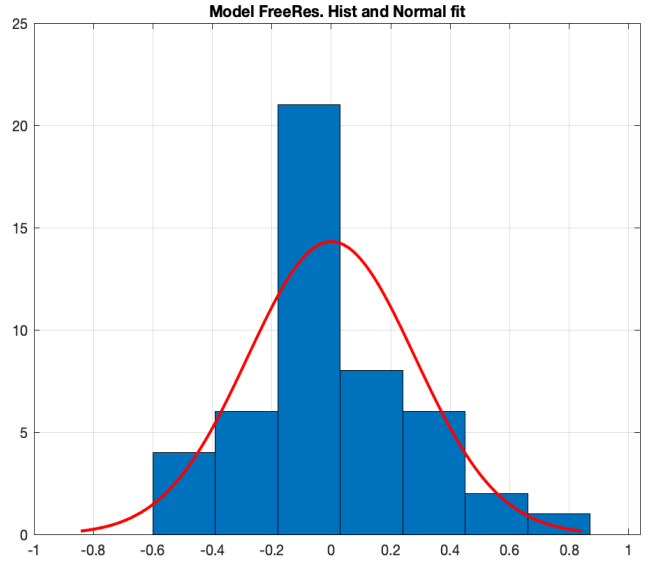


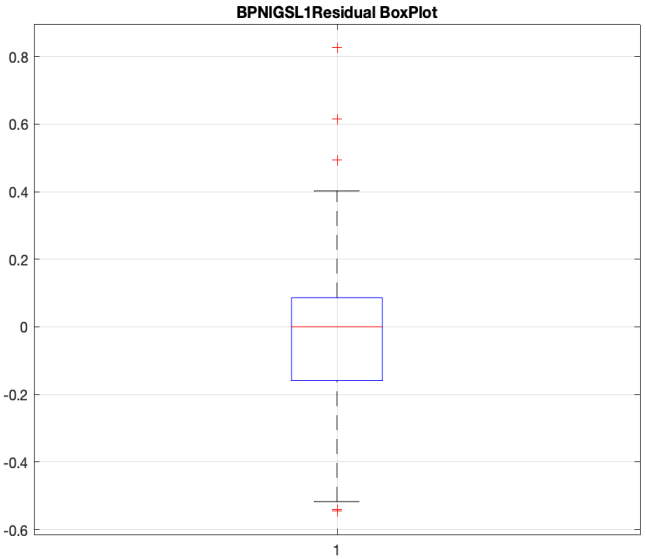
$\chi^2 = 7.889 \cdot 10^{-2}$
Computed parameters:

$$R_0 = 3.23, \quad C^{NH} = 5.66, \quad \tau_Q = 1.02$$

$$\Theta = 1.25, \quad \Phi = 0.86, \quad \nu_- = 2.1\text{MHz}, \quad \nu_+ = 2.8\text{MHz}$$

Statistical Analysis

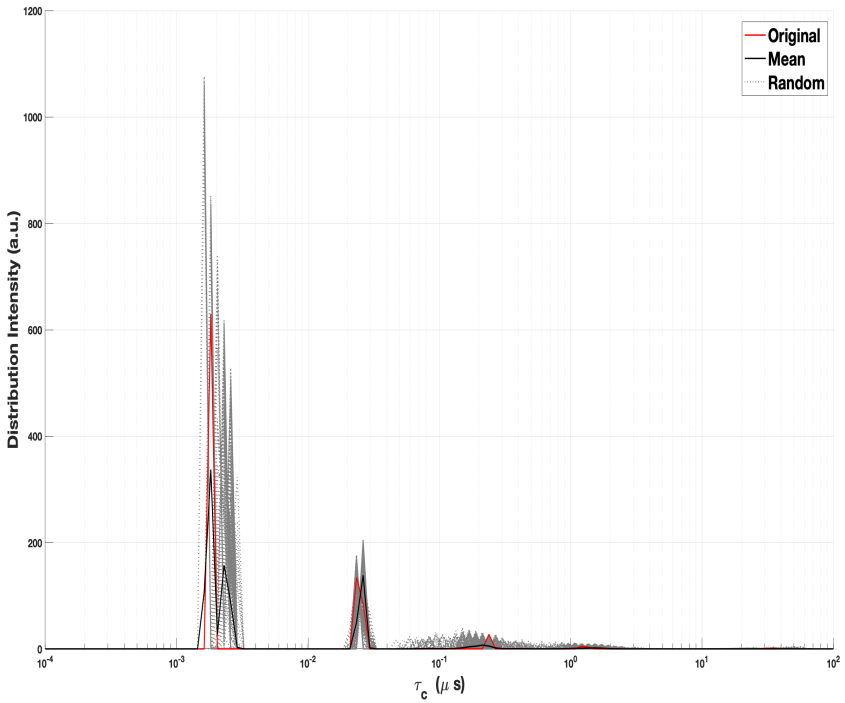




We apply the proposed method using 500 datasets obtained as

$$\boldsymbol{y}^{\boldsymbol{\delta}} = \boldsymbol{y} + \boldsymbol{\delta}$$

where $\boldsymbol{\delta}$ is a vector extracted with a random uniform distribution from the confidence intervals of the data.



MUPen2D

2D NMR relaxation data acquired using a conventional Inversion-Recovery (IR) experiment detected by a Carr-Purcell-Meiboom-Gill (IR-CPMG)[5] pulse train:

$$S(t_1, t_2) = \iint_0^\infty k_1(t_1, T_1) k_2(t_2, T_2) F(T_1, T_2)\ dT_1\ dT_2 + e(t_1, t_2) \qquad (9)$$

- S acquired data, at evolution times: t_1 in IR and t_2 in CPMG.
- $k_1(t_1, T_1) = 1 - 2e^{(-t_1/T_1)}$ and $k_2(t_2, T_2) = e^{(-t_2/T_2)}$
- $F(T_1, T_2)$ is the unknown distribution of longitudinal (T_1)and transverse (T_2) relaxation times.
- $F(T_1, T_2) \geq \ell$ where $\ell \in \mathbb{R}$.
- $e(t_1, t_2)$ represents additive noise, commonly modelled by a Gaussian distribution.

[5] B. Blumich. Essential NMR. Springer-Verlag, 2005.

Multipenalty Regularization[6]

$$\min_{\mathbf{f}} \left\{ \|\mathbf{K}\mathbf{f} - \mathbf{s}\|_2^2 + \sum_{i=1}^{N-1} \lambda_i (\mathbf{L}\mathbf{f})_i^2 + \alpha \|\mathbf{f}\|_1 \right\} \tag{10}$$

- $\mathbf{L}$ Discrete Laplacian Matrix
- $\lambda_i \geq 0, i = 1, \ldots, N-1$, locally adaptive L_2-regularization parameters
- $\alpha > 0$, L_1-regularization parameter.
- For fixed values λ_i and α, problem (10) can be written as:

$$\min_{\mathbf{f}} \{\Psi_1(\mathbf{f}) + \Psi_2(\mathbf{f})\}$$

$$\text{where } \Psi_1(\mathbf{f}) = \left\| \begin{pmatrix} \mathbf{K} \\ \sqrt{\Lambda}\mathbf{L} \end{pmatrix} \mathbf{f} - \begin{pmatrix} \mathbf{s} \\ \mathbf{0} \end{pmatrix} \right\|_2^2, \quad \Psi_2(\mathbf{f}) = \alpha \|\mathbf{f}\|_1, \ \Lambda = diag(\lambda_i)$$

Efficient Algorithm: **FISTA**

[6] V. Bortolotti, G. Landi, and F. Zama. 2DNMR data inversion using locally adapted multi-penalty regularization. *Computational Geosciences*, (25): 1215-1228, 2021.

Approximate Regularization Parameters

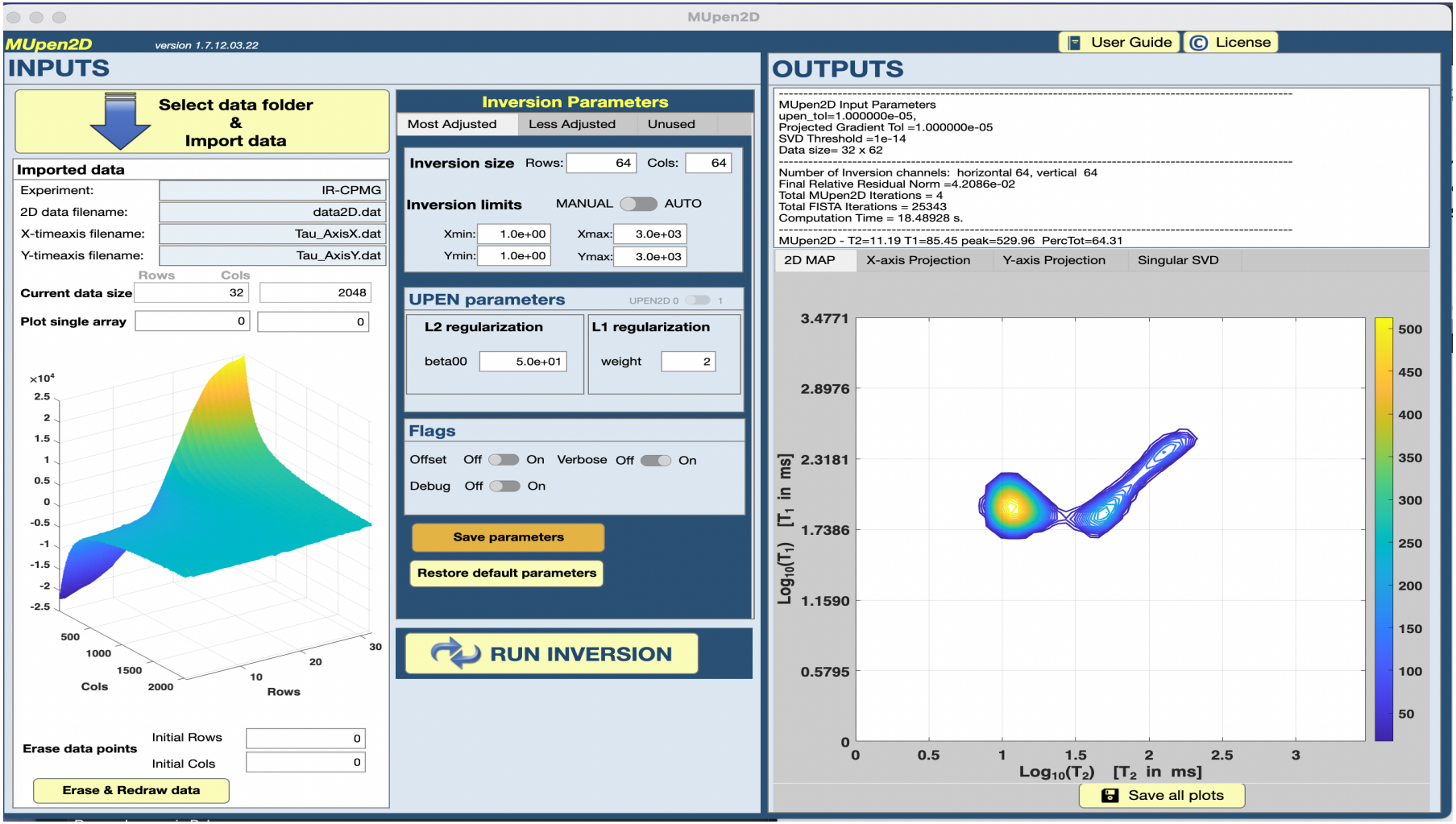
$$\alpha^{(n)} = \frac{\delta_n^2}{2\|\mathbf{f}^{(n)}\|_1} \tag{11}$$

$$\lambda_i^{(n)} = \frac{\delta_n^2}{2N\left(\beta_0 + \beta_p \mathcal{P}\left(\nabla\left(\mathbf{f}^{(n)}\right)\right)_i^2 + \beta_c \mathcal{P}\left(\boldsymbol{L}\mathbf{f}^{(n)}\right)_i^2\right)} \tag{12}$$

where

- $\mathbf{f}^{(n)}$ approximate solution, $\delta_n = \|\mathbf{K}\mathbf{f}^{(n)} - \mathbf{s}\|_2$
- $\beta_0 \simeq 10^{-5}$: threshold coefficient. $\beta_p = \beta_c = 1$ weights.
- $\mathcal{P}(\cdot)$ is the maximum filter of size 3×3

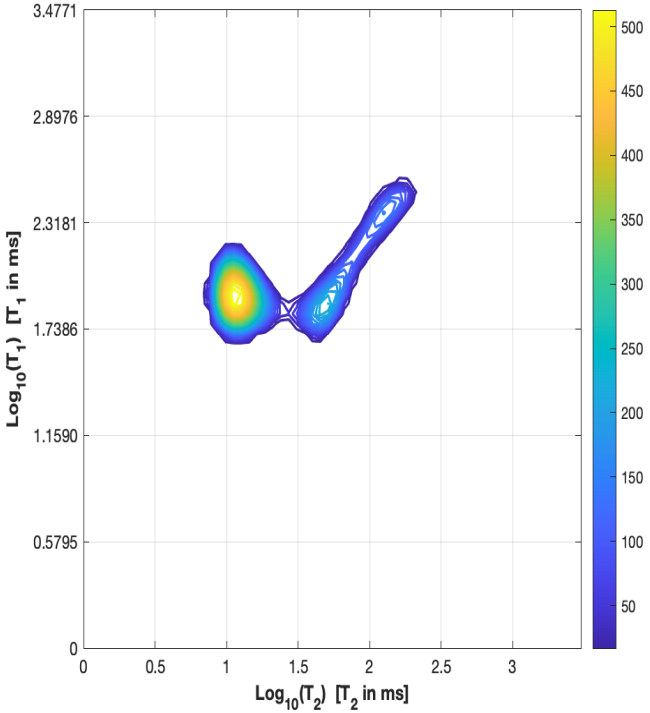
MUPen2D Software[7]

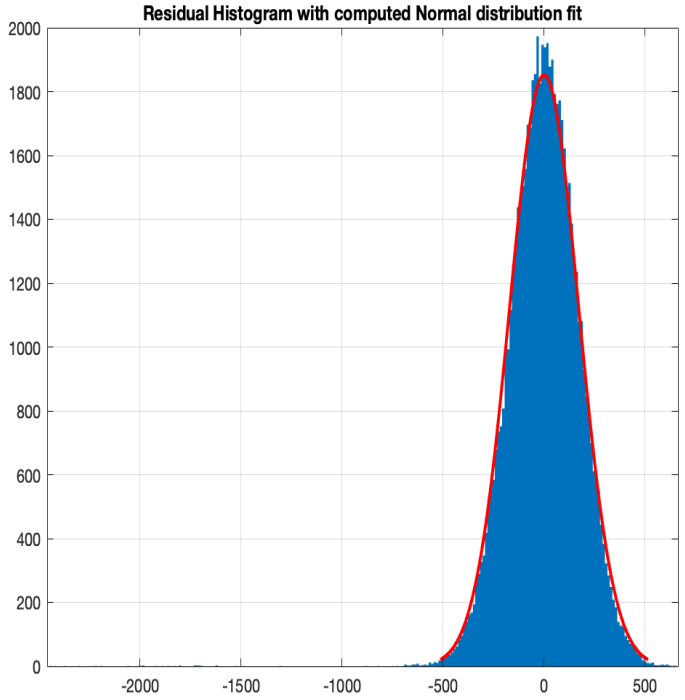


[7] https://site.unibo.it/softwaredicam/en/mupen2d

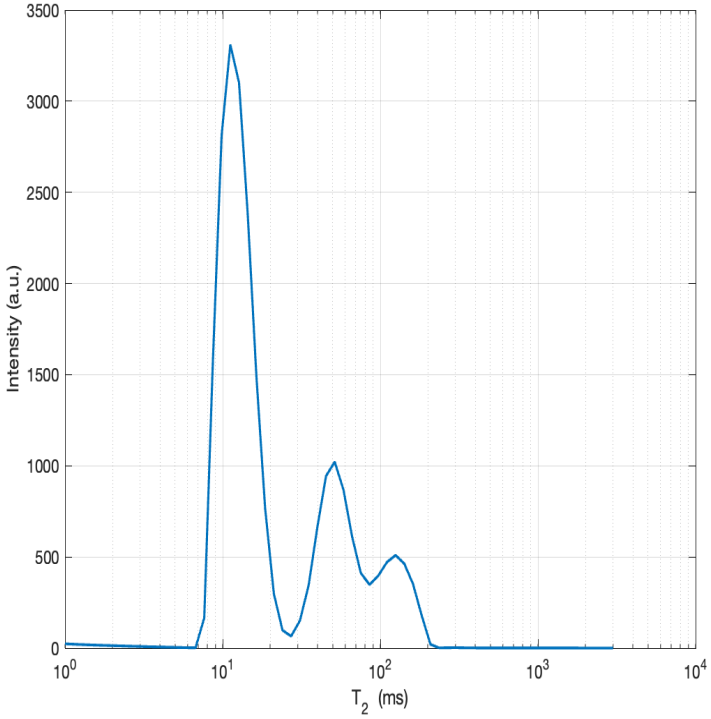
Results - Grana Padano cheese

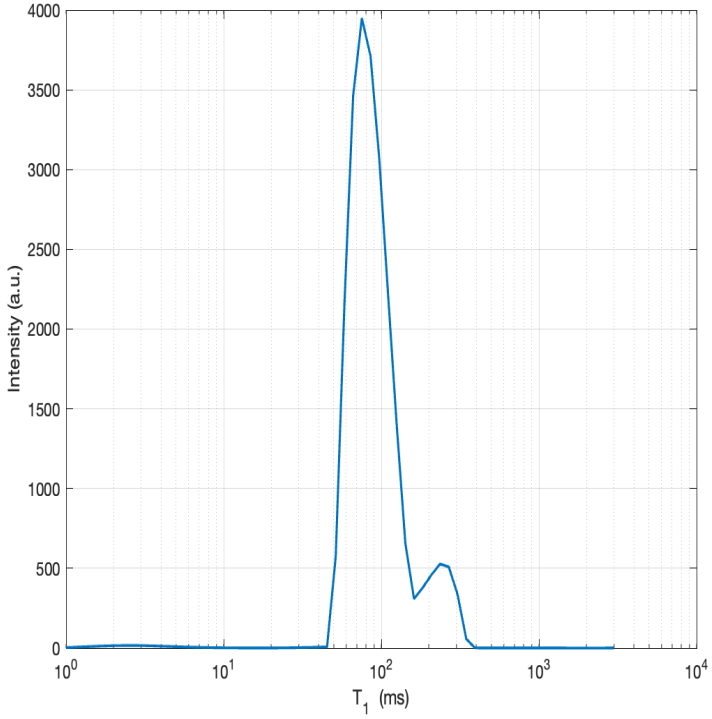
- Measurements have been performed on a Stelar SMARtracer Relaxometer at room temperature and using an Inversion Recovery CPMG sequence with 32 IR values and 2048 CPMG. Relaxation field: 7.2 MHz.
- T1-T2 maps computed by MUpen 2D Software Tool.





Results - 1D Distributions





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ModelFreeFFC

ModelFreeFFC is a freeware standalone Matlab® tool, developed at the University of Bologna (Bologna, Italy), with a graphical interface (GUI) for Windows, Linux OSs useful for fitting nuclear magnetic relaxation dispersion (NMRD) curves obtained by fast field cycling nuclear magnetic resonance (FFC-NMR) relaxometry measurements. The model used to fit the NMRD curve is supposed to be the "model free" one [1].

The Software is provided 'AS IS', without warranty of any kind, express or implied. In no event shall the copyright holder(s) be liable for any claim, data loss, loss of profits, damages or other liability arising from the Software's use or misuse. You use it at your own risk. Please read the License document for the terms of use ("License_ModelFree.pdf").

In addition to the compiled standalone GUI version (developed with the App Designer Matlab tool), there is also a standalone command- line executable version, both for Windows OS and Linux OS (See SOFTWARE INSTALLATION paragraph). The tool allows the user to handle some parameters that greatly influence the quality of the NMR maps and the computation time to perform the inversion. There is also a set of diagnostic tools that allow the user to evaluate the quality of the measured data. Remember that to have a good inversion, it is fundamental to have high-quality data (data without too many outliers or electronic baseline, relaxation curves not correctly sampled or distorted, etc.).

Reference

[1] P. Lo Meo, S. Terranova, A. Di Vincenzo, D. Chillura Martino and P. Conte. Heuristic Algorithm for the Analysis of Fast Field Cycling (FFC) NMR Dispersion Curves. Anal. Chem. 2021, 93, 24, 8553–8558. https://doi.org/10.1021/acs.analchem.1c01264.

ZIPPED FOLDER WITH EXECUTABLES AND DATA FOR WINDOWS OS

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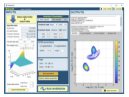
MUpen2D Software

MUpen2D a FREE multiple regularization Upen like tool for the inversion of 2D NMR data.



MUpen2D is a free two-dimensional (2D) inversion program software developed at the University of Bologna (Bologna, Italy), as an extension of the Upen2DTool that processes 2D ASCII Nuclear Magnetic Relaxation (NMR) data to produce distributions in the two NMR dimensions (2DNMR maps). At present, the following 2DNMR distribution maps are considered: T_1-T_2 longitudinal-transverse relaxation times, T_2-T_2 transverse-transverse relaxation times and D-T_2 diffusion - transverse relaxation times. MUpen2D implements the Multiple Uniform Penalty algorithm by extending the Uniform PENalty principle to two-dimensional data, including L1 norm and locally adapted L2 norm penalty terms. The algorithm produces the 2DNMR maps by solving a sequence of regularized least-squares problems. The regularization parameters are computed by an automatic update rule based on the Uniform Penalty principle. The software is written in Matlab® script language and it comes also with a standalone command line executable version and a compiled standalone graphical interface version, developed with App Designer, both for Windows OS and Linux OS. To perform the inversion the tool allows the user to handle some parameters that greatly influence the quality of the 2DNMR maps and also the computation time. There is also a set of diagnostic tools that allows the user to evaluate the quality of the measured data. Remember that in order to have a good inversion it fundamental to have high quality data (data without too many outliers or electronic baseline, relaxation curves correctly sampled or distorted, etc…).

To run the executables it is necessary to install the appropriate Matlab library, the present releases have been developed with MatLab 2020b.

ZIPPED FOLDER WITH EXECUTABLES AND DATA FOR WINDOWS OS

MUpen2D for Windows OS [.zip 7780Kb]

Unzip the file to obtain the executable version of MUpen2D (both Command line and Graphical version) and a set of data.

ZIPPED FOLDER WITH EXECUTABLES AND DATA FOR LINUX OS

Zipped Folder with Executables and Data [.zip 6840Kb]

Unzip the file to obtain the executable version of MUpen2D (both Command line and Graphical version) and a set of data.

LICENSE

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MANUAL WITH INSTALLATION GUIDE

MUpen2D draft manual [.pdf 1362Kb]

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Thank for your attention!