Algorithmes pour rechercher la phase des diagrammes de diffraction cohérentes

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Journée Scientifique sur
Diffraction et Diffusion
des X Coherents
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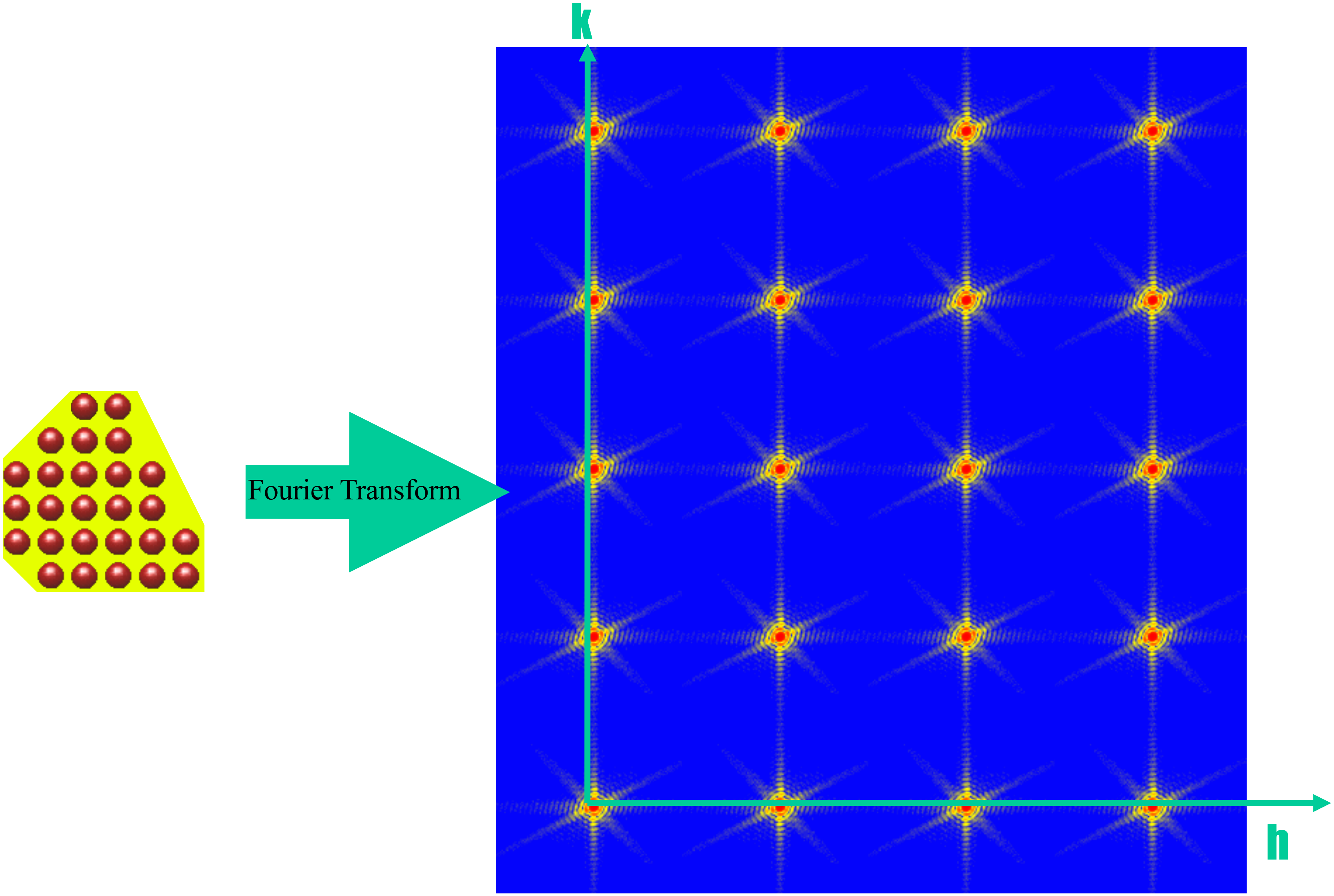
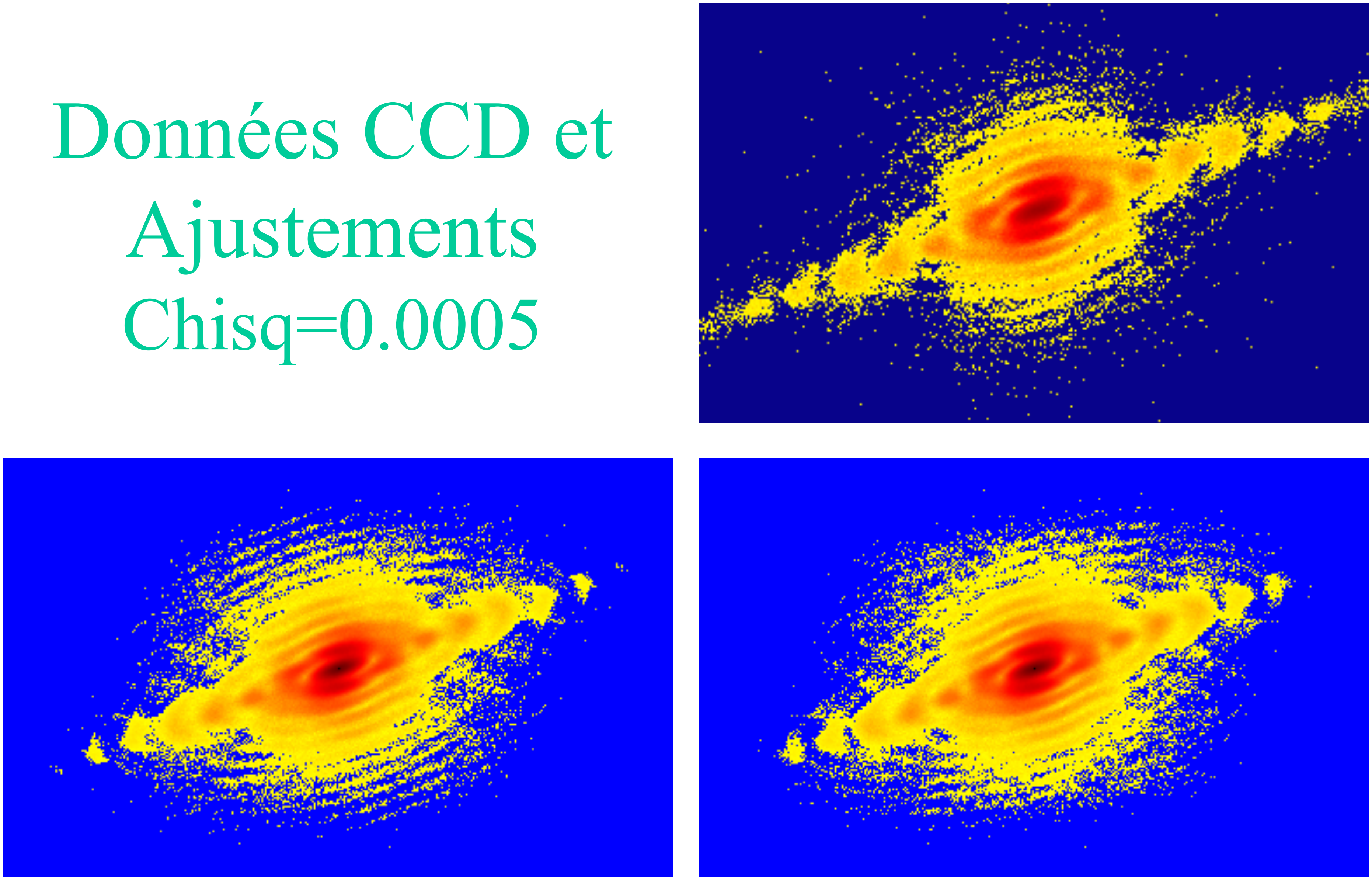
Resumé

- Taille des Nanocristaux
- Unicité
- Algorithmes
- Convergence
- Vortices
- Sommaire

Diffusion cohérente des Cristaux

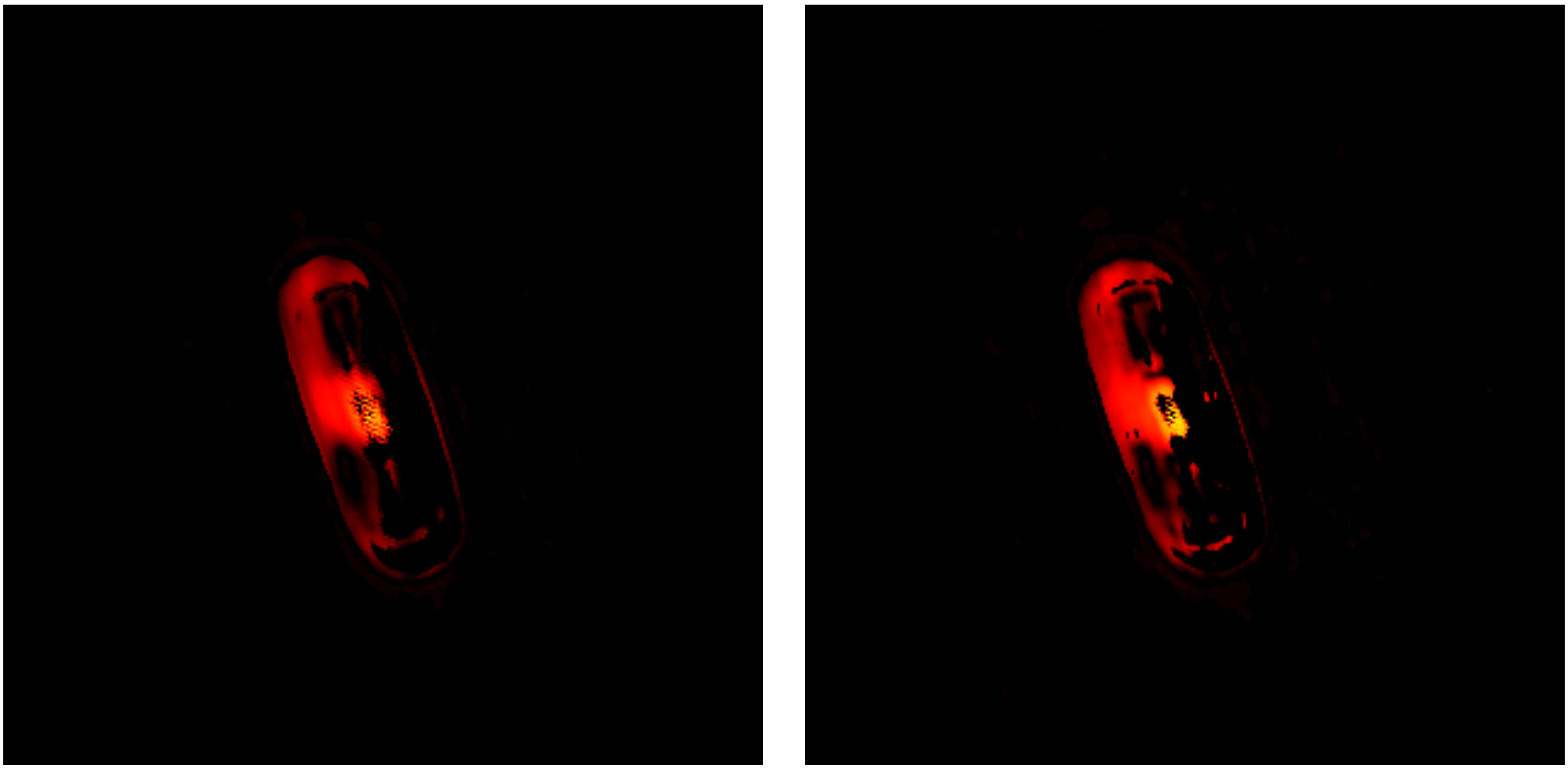


Données CCD et Ajustements Chisq=0.0005

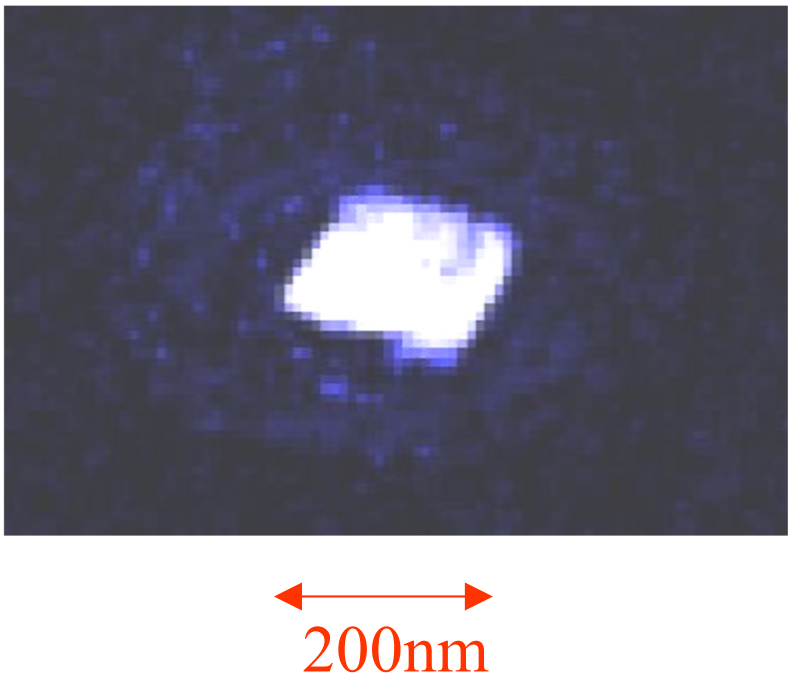


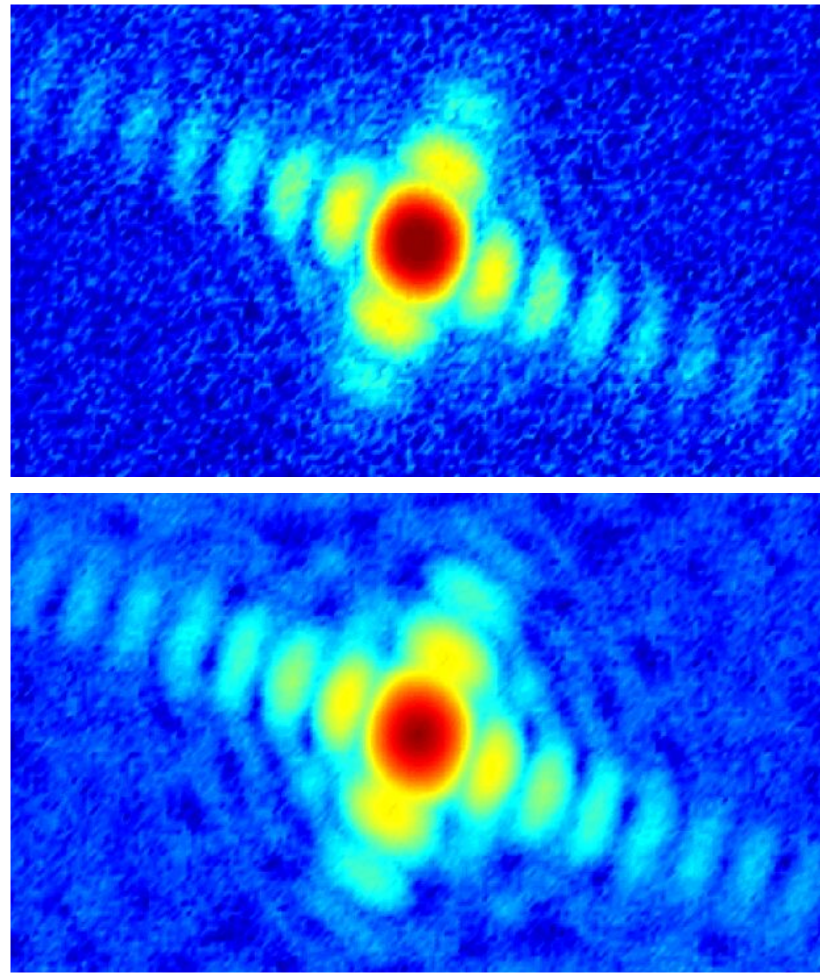
2D Reconstructions

chisquare = 0.0005



Reconstruction of Ag Nanocrystal





Unicité (uniqueness) par Convolution

In contrast, if we take two functions of with compact support, $f(z)$ and $g(z)$, then their convolution is

$$h(z) = f(z) \otimes g(z) \tag{1.37}$$

and we may compose a second function

$$h'(z) = f(z) \otimes g^*(-z). \tag{1.38}$$

l via Hadamard's product:

$$F(k) = \prod_n a_n (k - k_n)^n. \tag{1.40}$$

Demonstration de Uniqueness

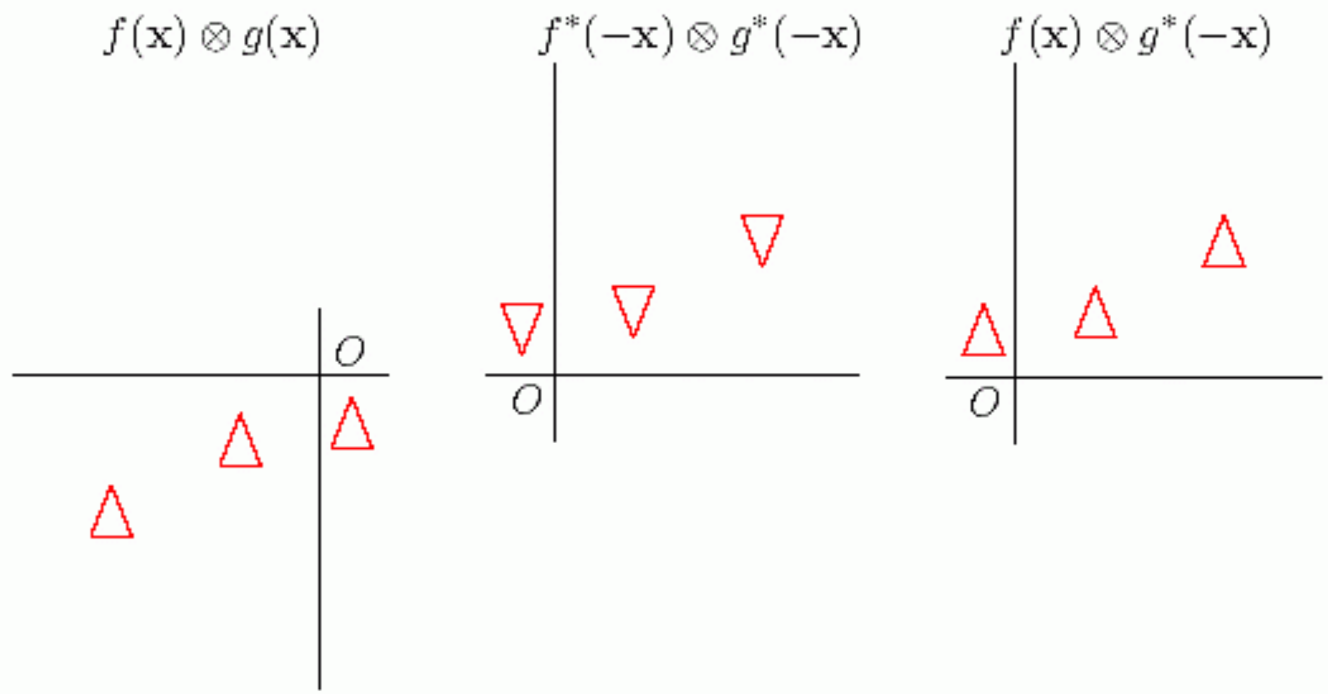
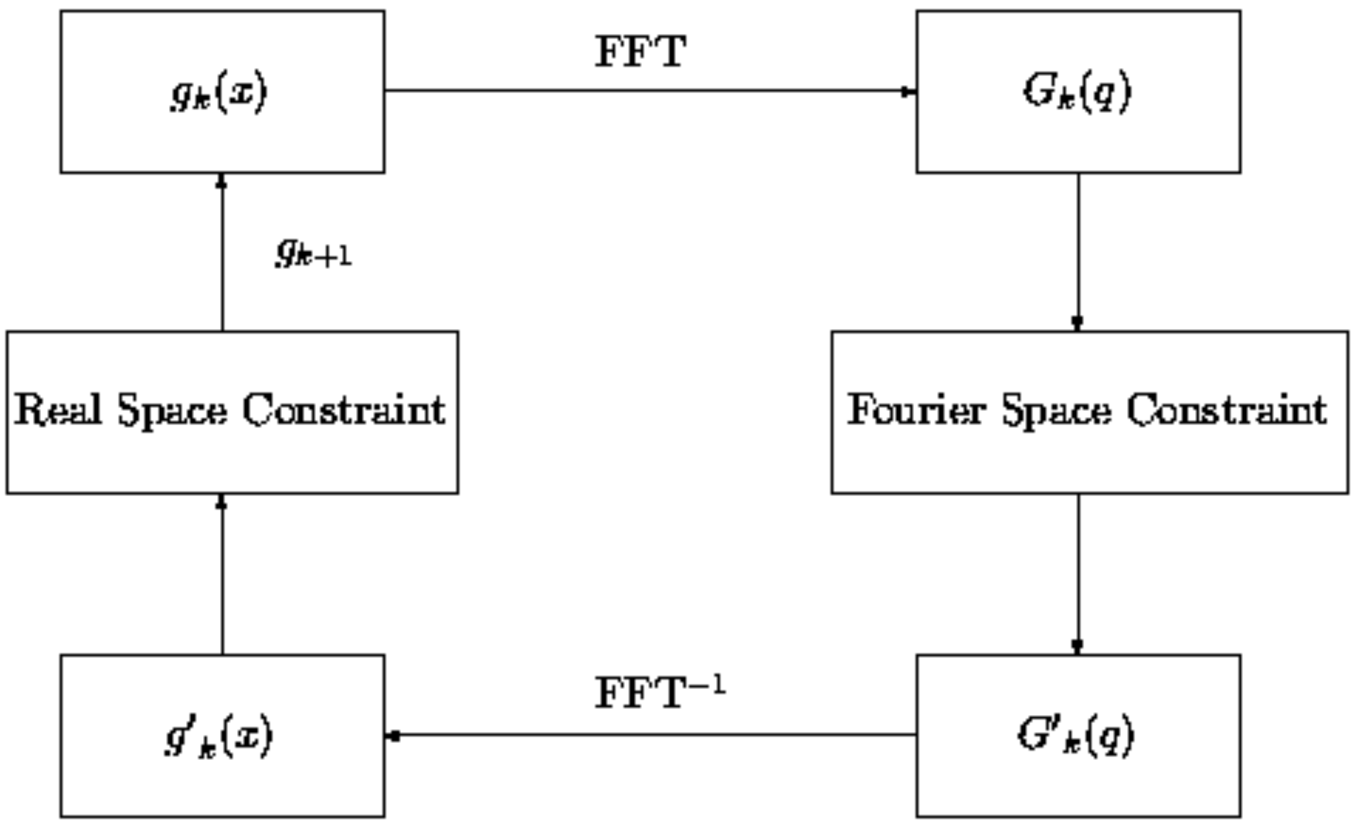


Figure 1.1: All three examples have the same Fourier magnitude, demonstrating that ambiguous solutions are possible in 2D. $f(\mathbf{x})$ is the shape of the triangle. $g(\mathbf{x}) = \delta(\mathbf{x}-\mathbf{x_1}) + \delta(\mathbf{x}-\mathbf{x_2}) + \delta(\mathbf{x}-\mathbf{x_3})$, where the vectors $\mathbf{x_i}$ are from the origin to the center of each triangle. The leftmost two are the "correct" solution and its twin–a trivial ambiguity–while the third demonstrates that if $|F(\mathbf{k})||G(\mathbf{k})|$ can be factorized an ambiguous solution may exist.

Chapitre 2: Algorithmes

Generic “Error Reduction” method



Methode Gerchberg-Saxton (GS)

R. W. Gerchberg and W. O. Saxton Optik 35 237 (1972)

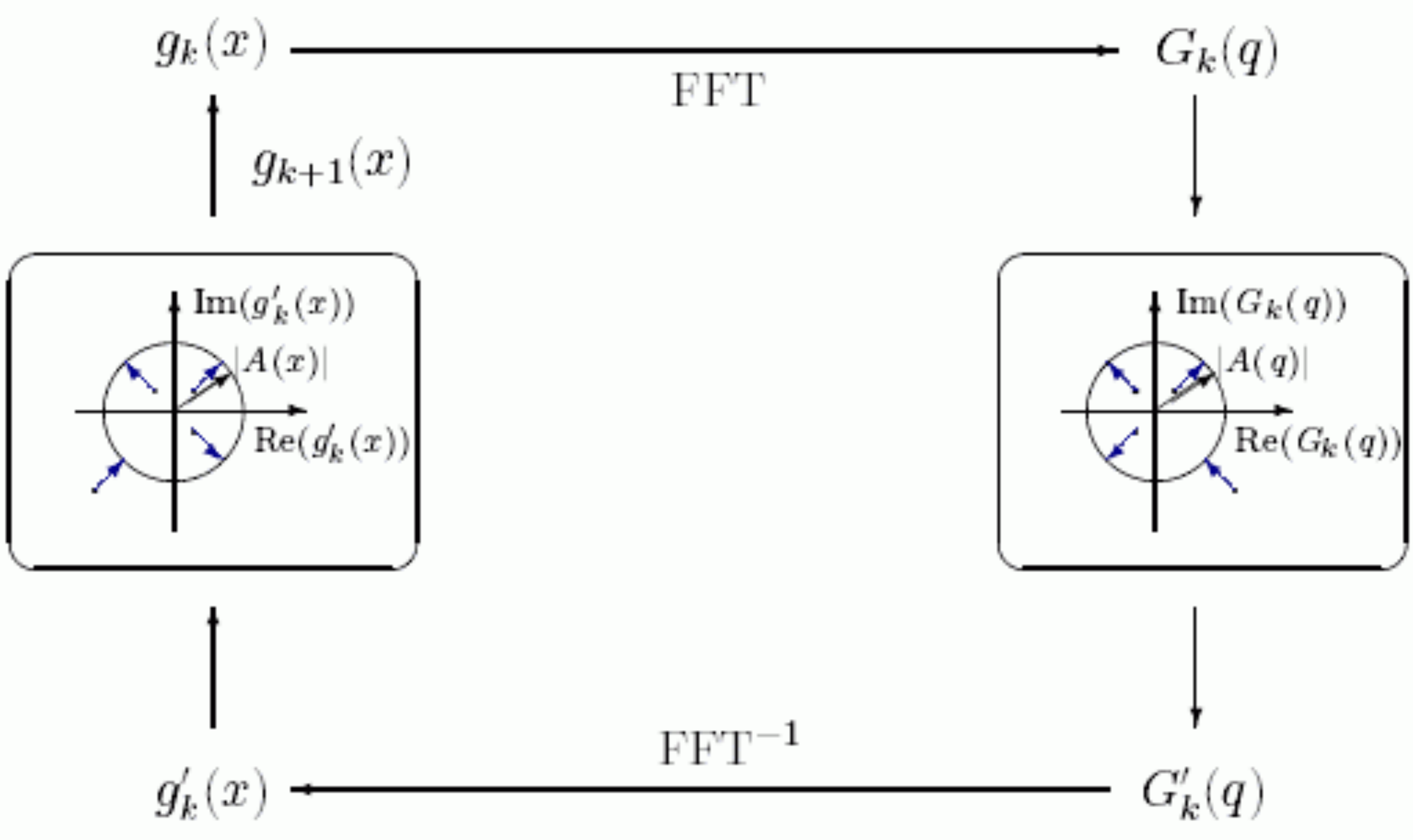


Figure 2.1: Gerchberg-Saxton Algorithm.

Methode du Reduction d'Erreur (ER)

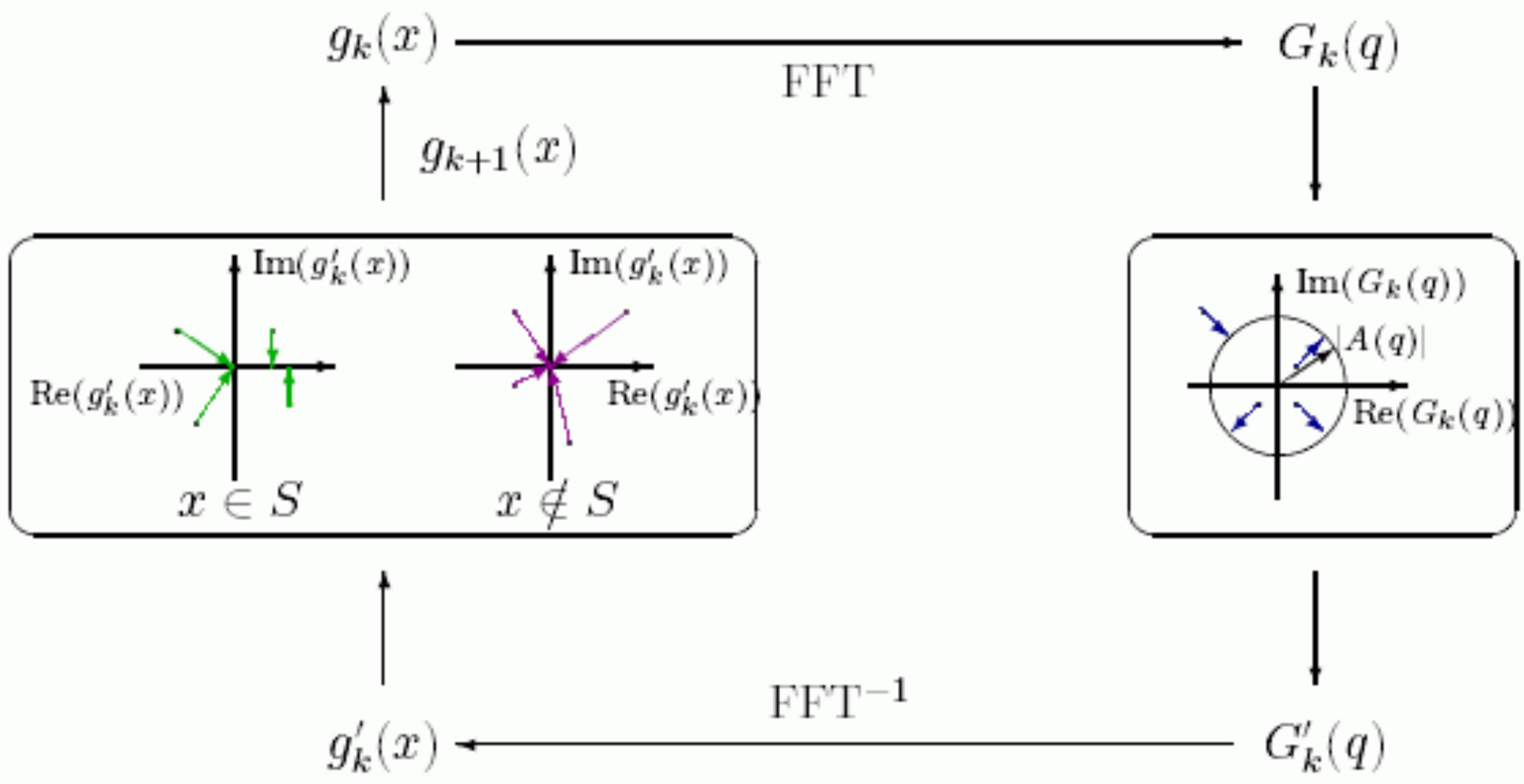


Figure 2.2: Error Reduction Algorithm.

Methode HIO de Fienup

J. R. Fienup Appl. Opt. 21 2758 (1982)

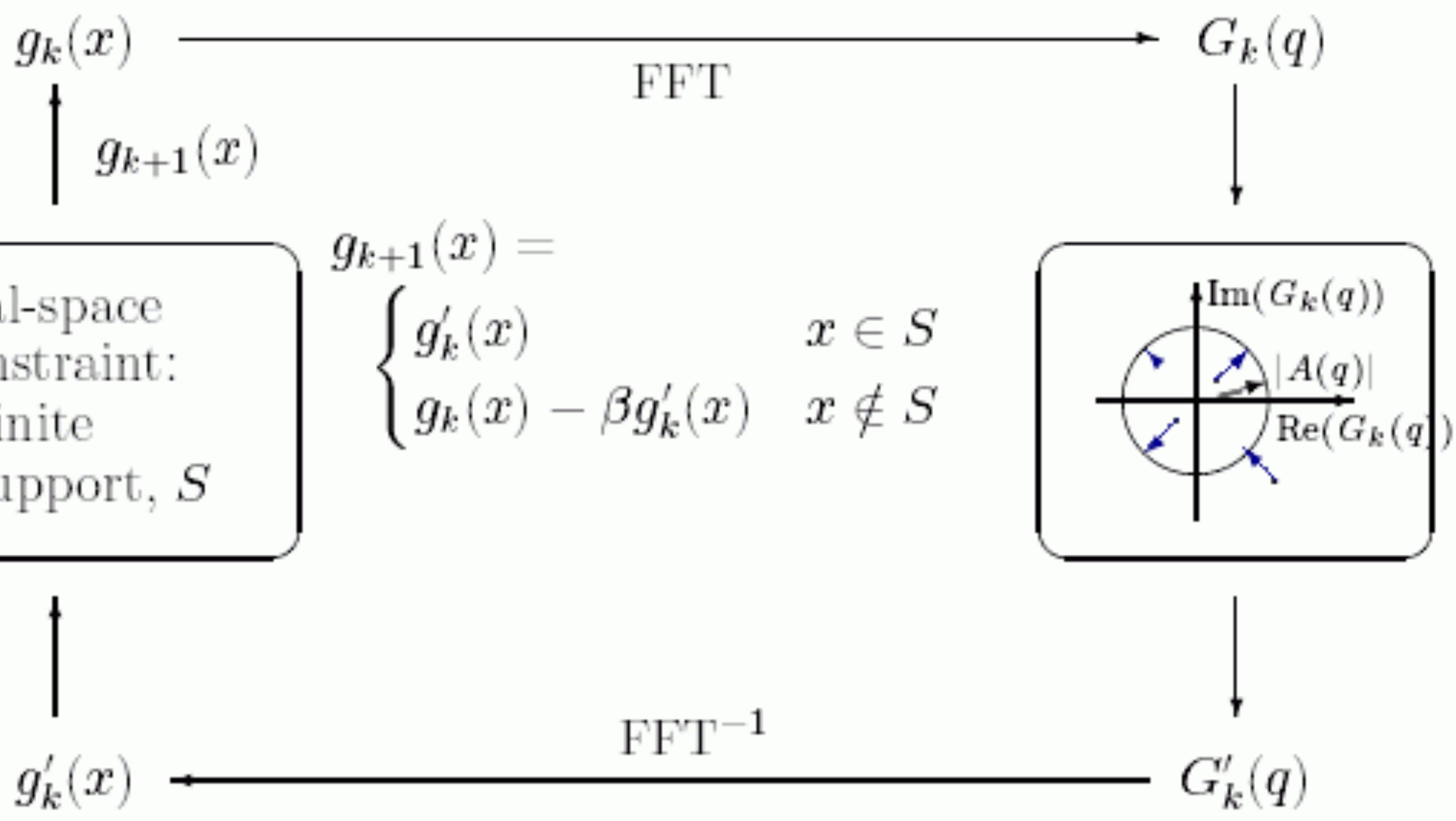


Figure 2.3: Fienup HIO

Version HIO de Millane

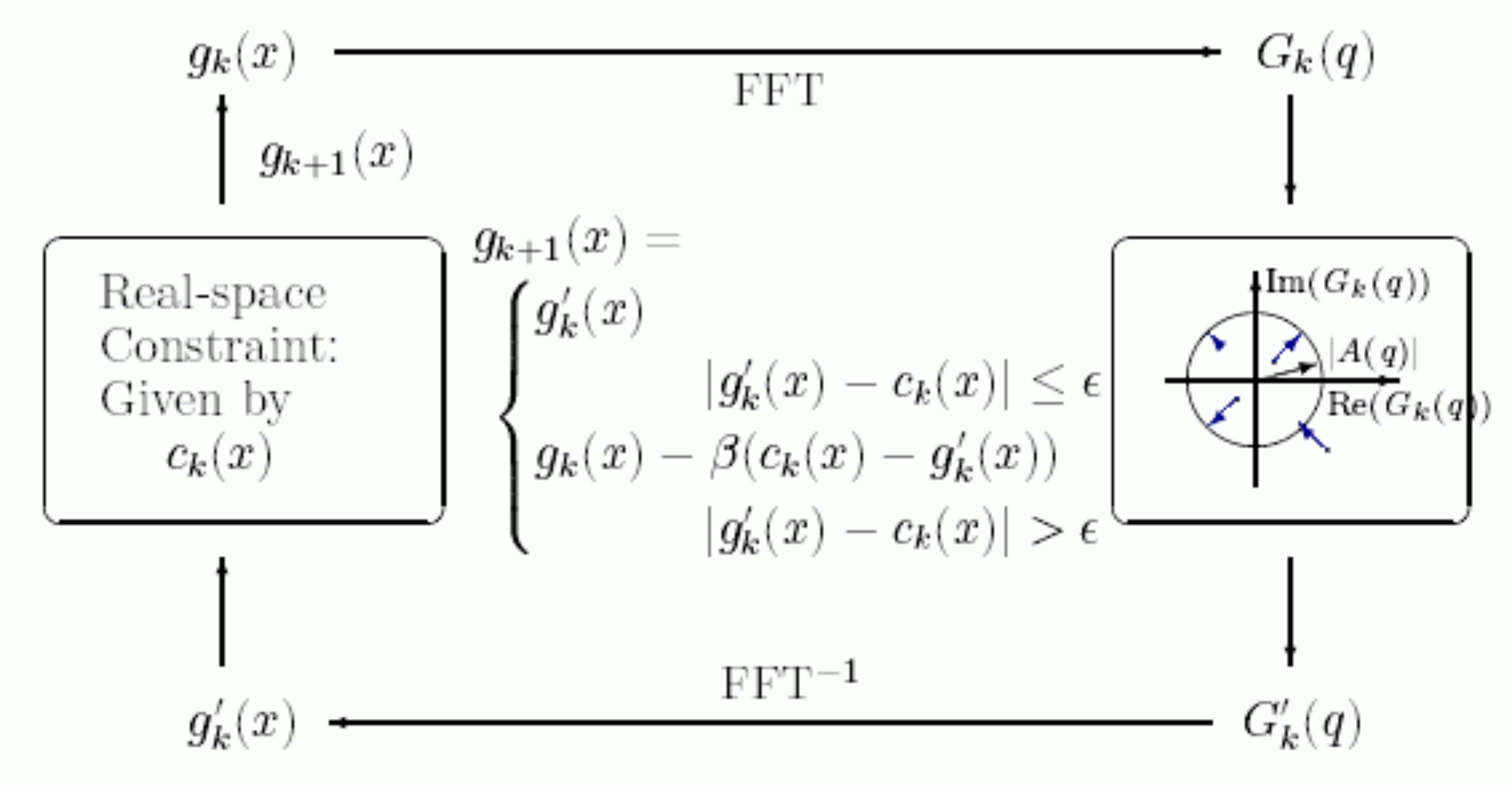


Figure 2.4: Millane's HIO.

Variations de "Hybrid Input-Output"

$$g_{k+1} = \begin{cases} g'_k & \text{if } x \in S \\ 0 & \text{if } x \notin S \end{cases} . \qquad (2.7)$$

Reduction d'erreur

$$\begin{aligned} g_{k+1}(x) &= g_k(x) + \beta \Delta g_k(x) \\ &= \begin{cases} g_k(x) & \text{if } x \in S \\ g_k(x) - \beta g'_k(x) & \text{if } x \notin S \end{cases} . \end{aligned} \qquad (2.20)$$

IO "basique"

$$g_{k+1}(x) = \begin{cases} g'_k(x) & \text{if } x \in S \\ g_k(x) - \beta g'_k(x) & \text{if } x \notin S \end{cases} , \qquad (2.22)$$

HIO Fienup

HIO Millane

$$g_{k+1}(x) = \begin{cases} g'_k(x) & \text{if } |c_k(x) - g'_k(x)| \leq \epsilon \\ g_k(x) - \beta\left(g'_k(x) - c_k(x)\right) & \text{if } |c_k(x) - g'_k(x)| > \epsilon \end{cases} , \qquad (2.23)$$

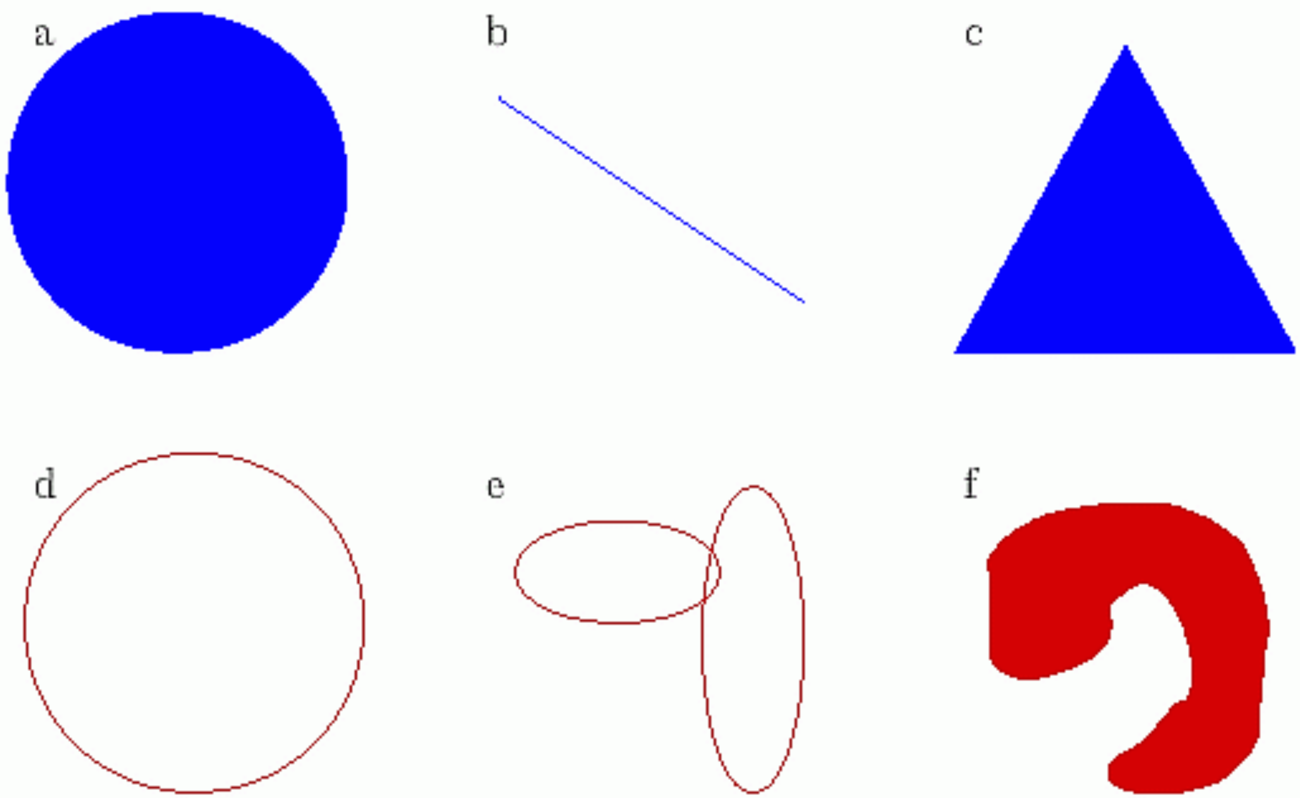


Figure 2.5: a) a filled disk, b) a 1D line, c) a filled triangle, d) a circle,e) two intersecting circles, f) a crescent-like shape. The colored region indicates the extent of the set. The first three(a-c) sets are convex, because the shortest line segment joining any two points within the set lies entirely within the set. The last three(d-f) sets are nonconvex, because the shortest line segments joining any two points within the set contains at least one point outside the set.

Ensembles Convexes

Ensembles Non-convexes

Trajectoire de l'Algorithme ER

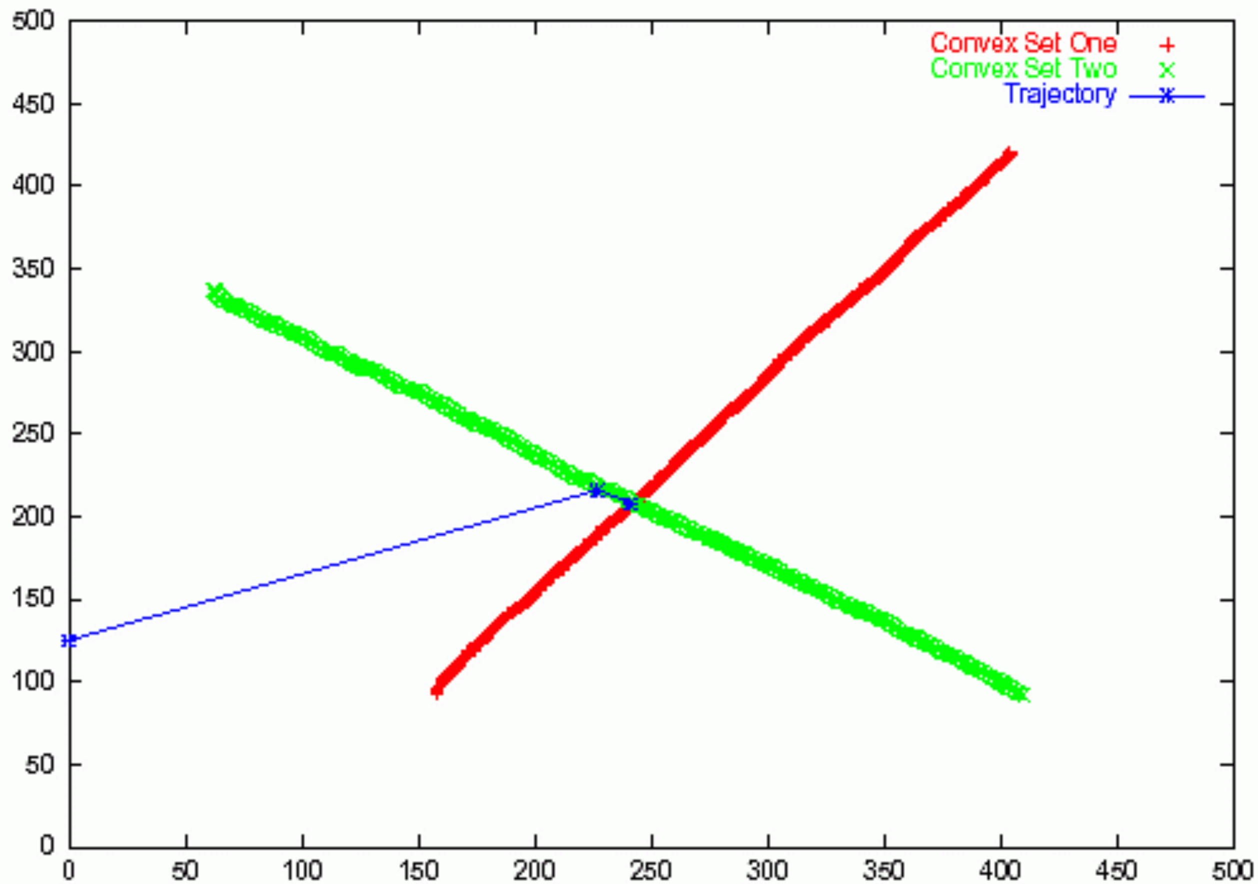


Figure 2.6: Trajectory of GS/ER. Because these two are alternating projection algorithms, the iterate will follow the contour of the boundary of a set.

Trajectoire de l'Algorithme HIO

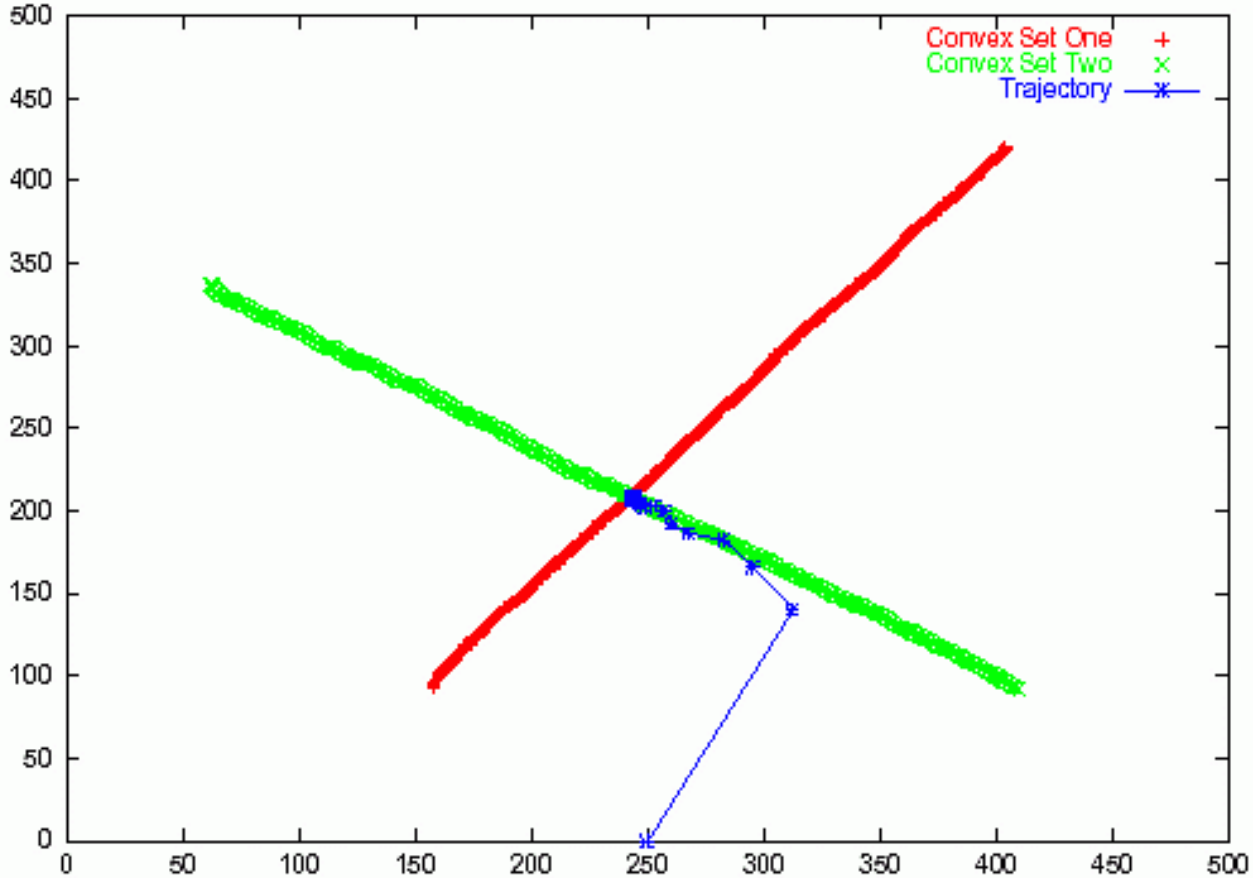


Figure 2.7: Trajectory of HIO. HIO does not follow the contour of the set as strictly as GS/ER. It has a tendency to spiral inward toward the intersection. For this example, $\beta = 0.3$ has been chosen so that the step size is short and therefore better illustrates this behavior.

Methode de Projections

$$\rho_{n+1} = (\pi_{m(o)} \pi_{m(i)}) \rho_n. \tag{2.24}$$

Alg GS

$$\rho_{n+1} = (\pi_s \pi_+ \pi_m) \rho_n = (\pi_{s+} \pi_m) \rho_n, \tag{2.25}$$

Alg ER

$$\rho_{n+1}(u) = \begin{cases} \pi_m \rho_n(u) & \text{if } u \in S \\ (1 - \beta \pi_m) \rho_n(u) & \text{if } u \notin S \end{cases}, \tag{2.26}$$

Alg HIO

$$\begin{aligned} \rho_{n+1} &= \pi_s \pi_m \rho_n + (1 - \pi_s)(1 - \beta \pi_m) \rho_n \\ &= \pi_s \pi_m \rho_n + \rho_n - \beta \pi_m \rho_n - \pi_s \rho_n + \beta \pi_s \pi_m \rho_n \\ &= \left[1 + (1 + \beta) \pi_s \pi_m - \pi_s - \beta \pi_m\right] \rho_n. \end{aligned} \tag{2.27}$$

Traitement de Veit Elser (Cornell): "Carte des Differences" = DM

$$\rho_{n+1} = D\rho_n = (1 + \beta\Delta)\rho_n = [1 + \beta\,(\pi_1 f_2 - \pi_2 f_1)]\rho_n, \tag{2.28}$$

$$f_i = (1 + \gamma_i)\pi_i - \gamma_i, \tag{2.30}$$

Mode I: γ_1=-1 γ_2=1/β DM = HIO (Fienup)

Mode II: γ_1=-1/β γ_2=1/β "maximally contractive"

Trajectoire de l'Algorithme DM

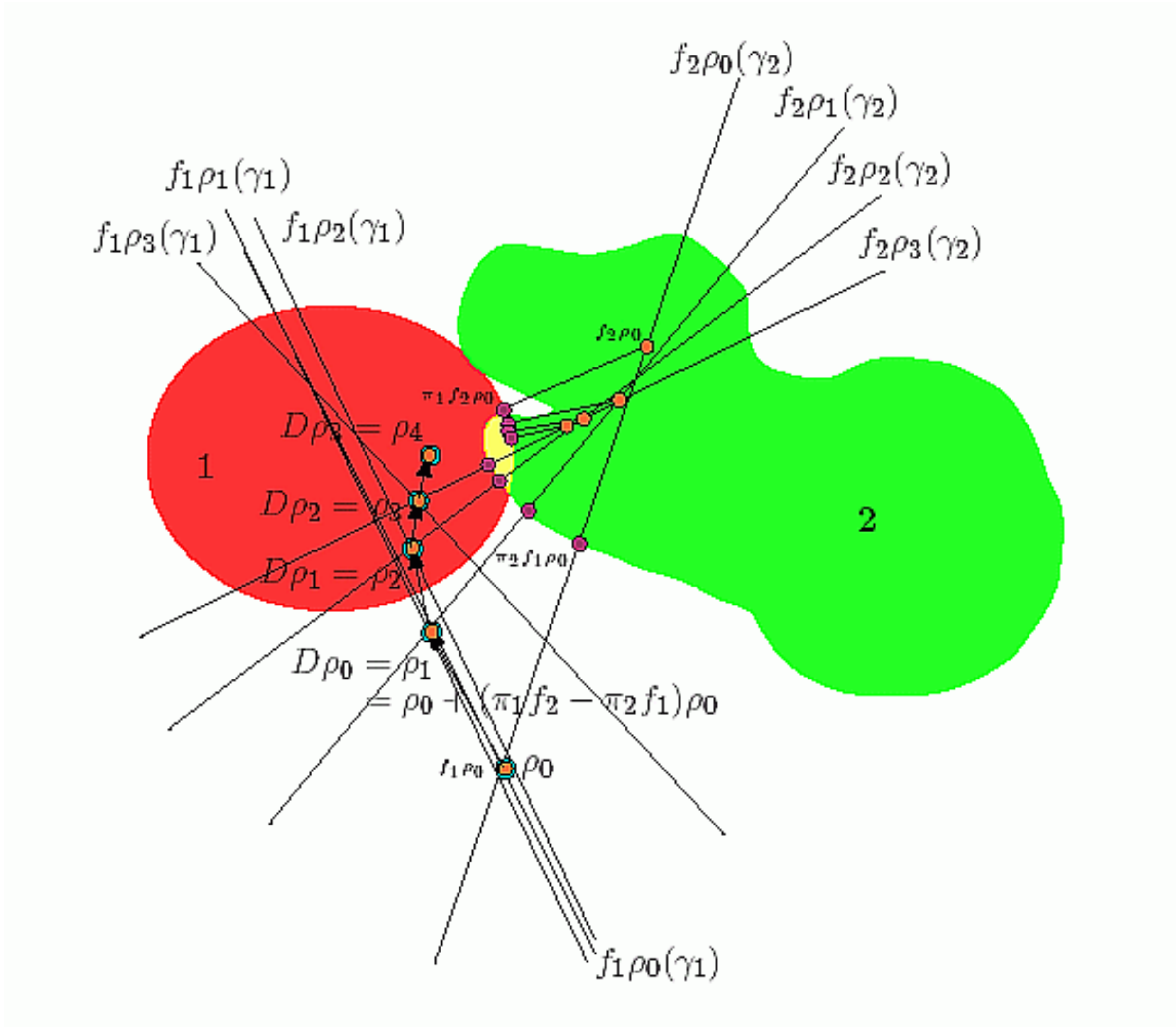
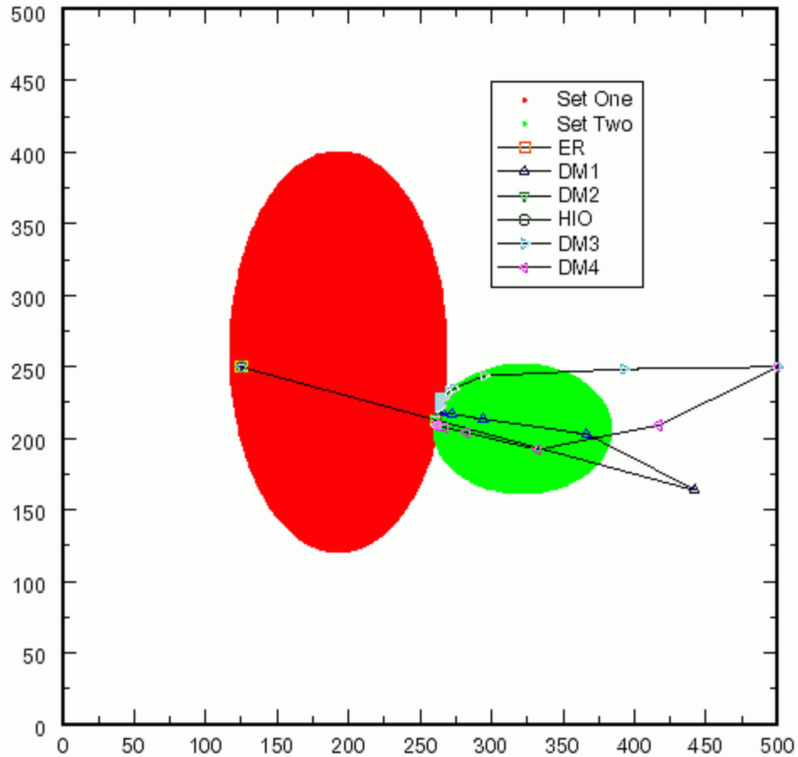
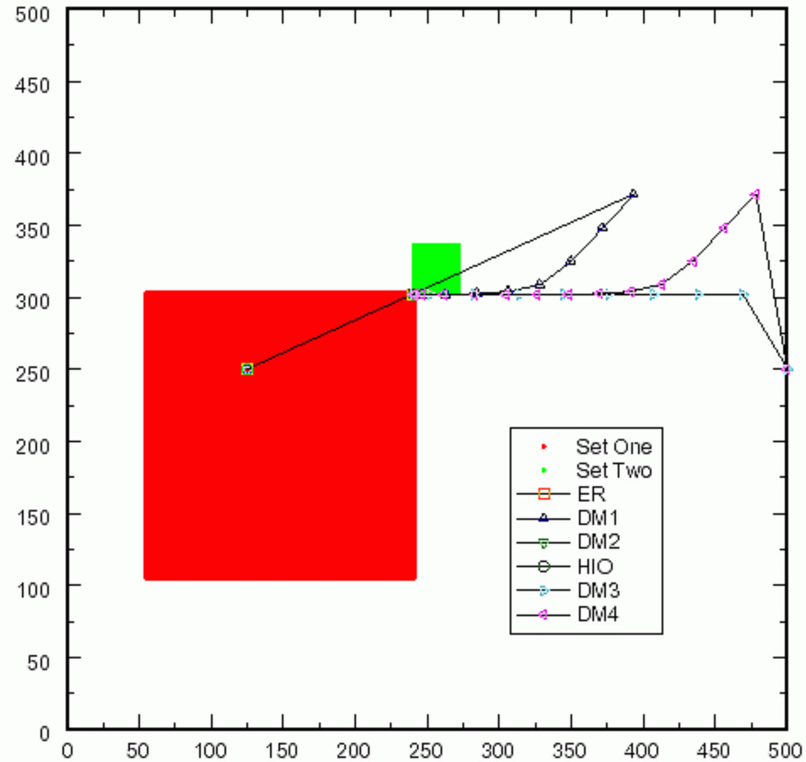


Figure 2.8: The trajectory of DM with $\beta = 1$, $\gamma_1 = -1$, and $\gamma_2 = 1$. With this choice of parameters, the DM is maximally contractive and corresponds to Fienup's HIO with $\beta = 1$. $f_i\rho_0(\gamma_i)$ is the line connecting ρ_0 with $\pi_i\rho_0$

Trajectoires d'Algorithme

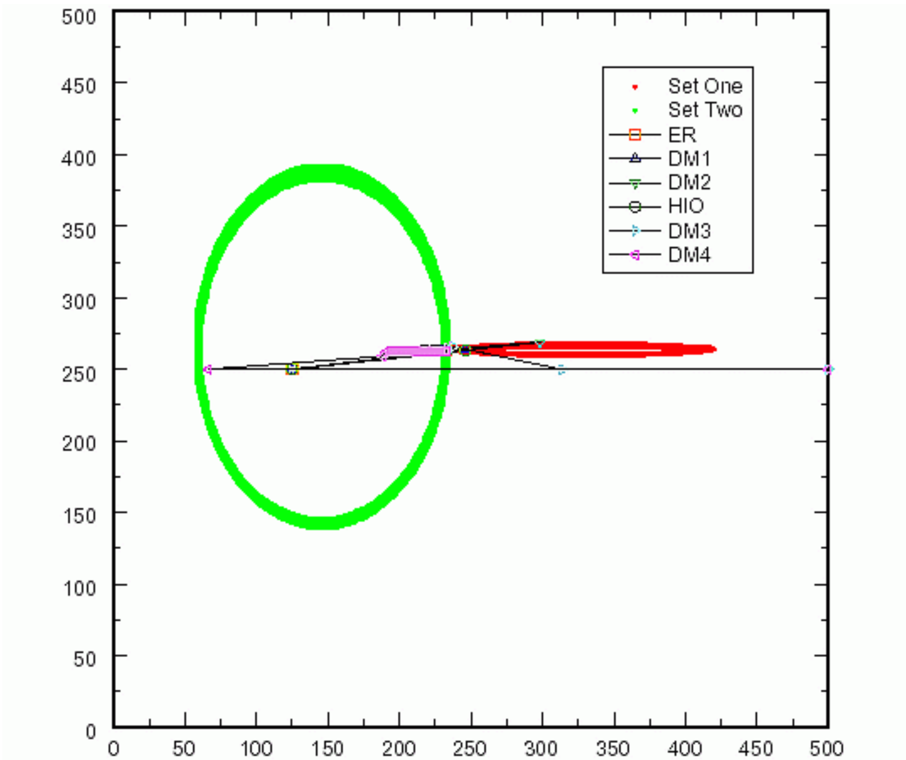


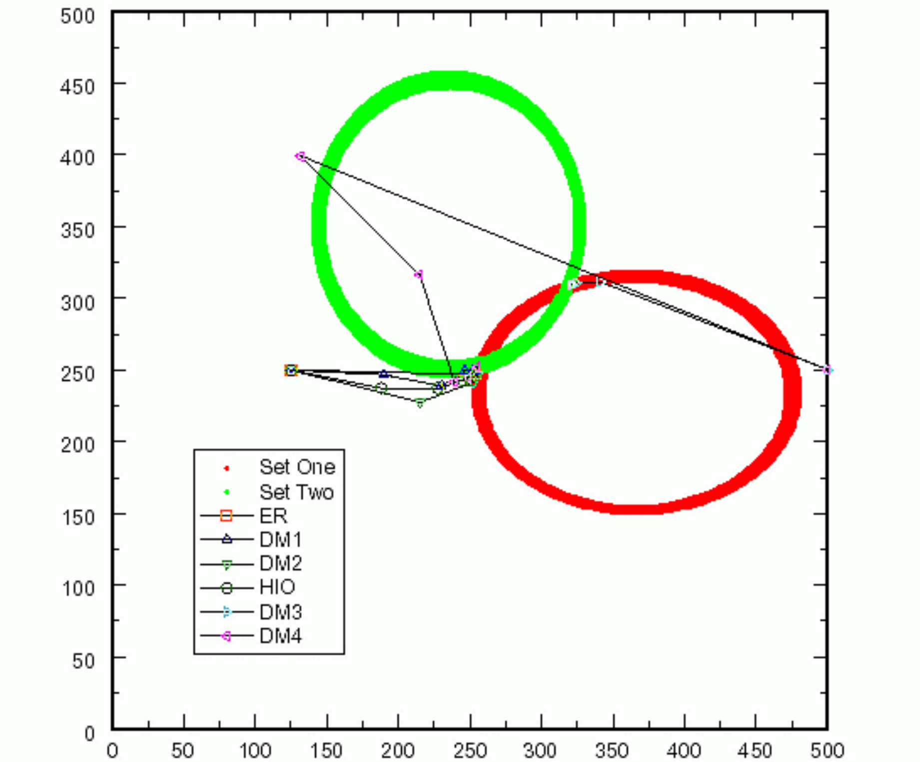


Label	Algorithm	Start x	Start y	Iterations	β	γ_1	γ_2
ER	ER	125	250	50	–	–	–
DM1	DM	125	250	50	0.7	-1	3.33
DM2	DM	125	250	50	0.7	-1.43	1.43
HIO	DM	125	250	50	0.7	-1	1.43
DM3	DM	500	250	50	0.1	-10	10
DM4	DM	500	250	50	0.7	-1	3.33

Label	Algorithm	Start x	Start y	Iterations	β	γ_1	γ_2
ER	ER	125	250	50	–	–	–
DM1	DM	125	250	50	0.7	-1	3.33
DM2	DM	125	250	50	0.7	-1.43	1.43
HIO	DM	125	250	50	0.7	-1	1.43
DM3	DM	500	250	50	0.1	-10	10
DM4	DM	500	250	50	0.7	-1	3.33

Trajectoires d'Algorithme

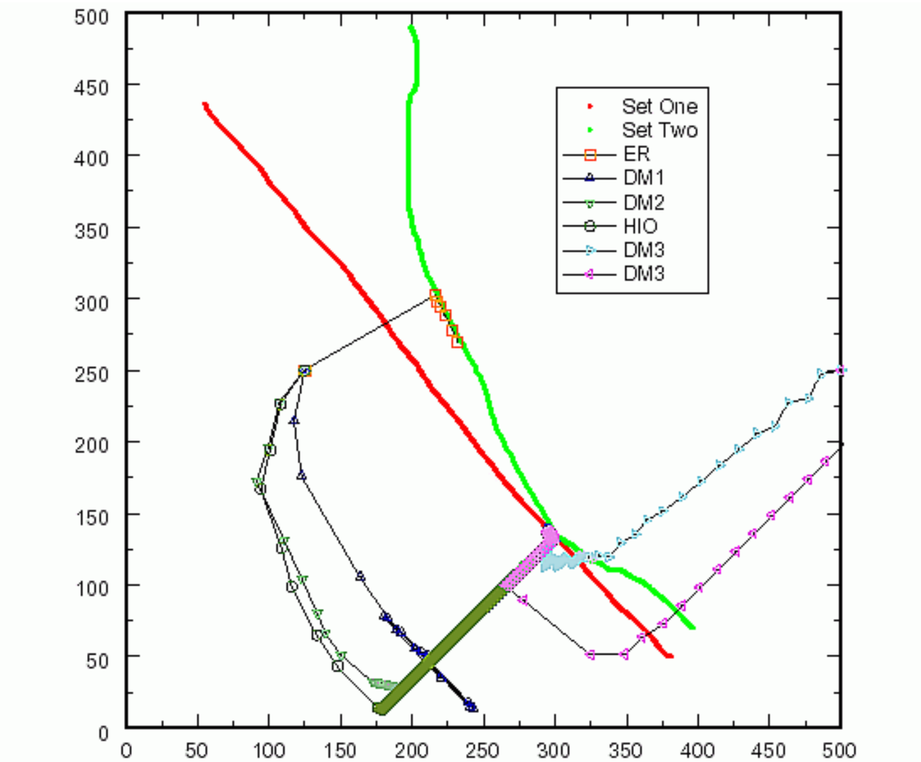


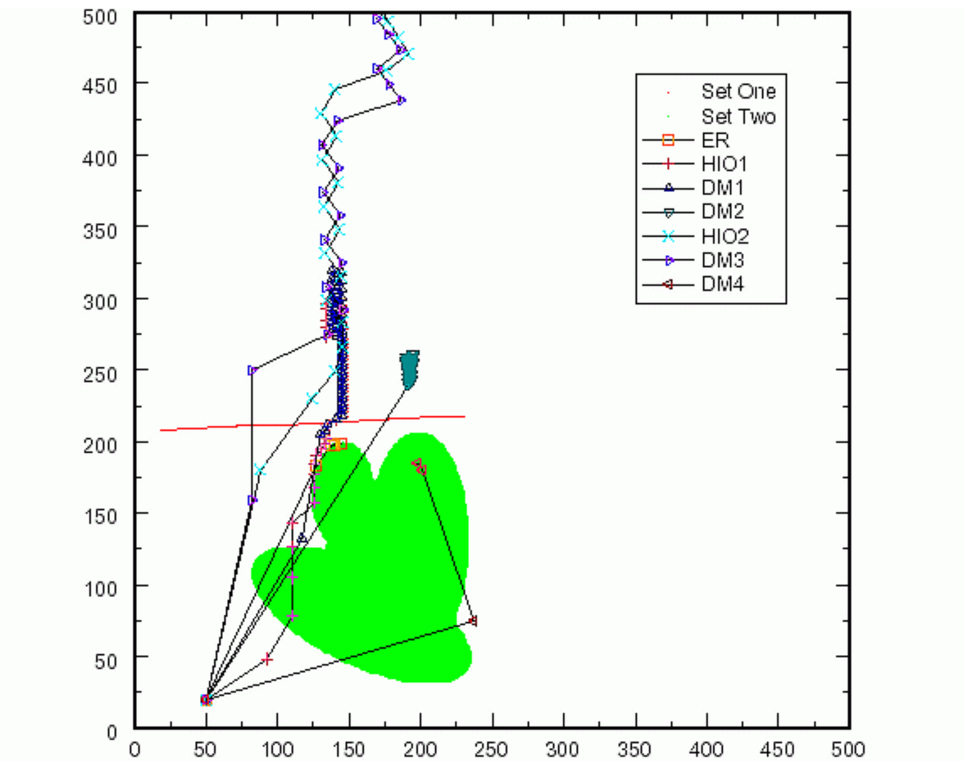


Label	Algorithm	Start x	Start y	Iterations	β	γ_1	γ_2
ER	ER	125	250	50	–	–	–
DM1	DM	125	250	50	0.7	-1	3.33
DM2	DM	125	250	50	0.7	-1.43	1.43
HIO	DM	125	250	50	0.7	-1	1.43
DM3	DM	500	250	50	0.1	-10	10
DM4	DM	500	250	50	0.7	-1	3.33

Label	Algorithm	Start x	Start y	Iterations	β	γ_1	γ_2
ER	ER	125	250	50	–	–	–
DM1	DM	125	250	50	0.7	-1	3.33
DM2	DM	125	250	50	0.7	-1.43	1.43
HIO	DM	125	250	50	0.7	-1	1.43
DM3	DM	500	250	50	0.1	-10	10
DM4	DM	500	250	50	0.7	-1	3.33

Trajectoires d'Algorithme

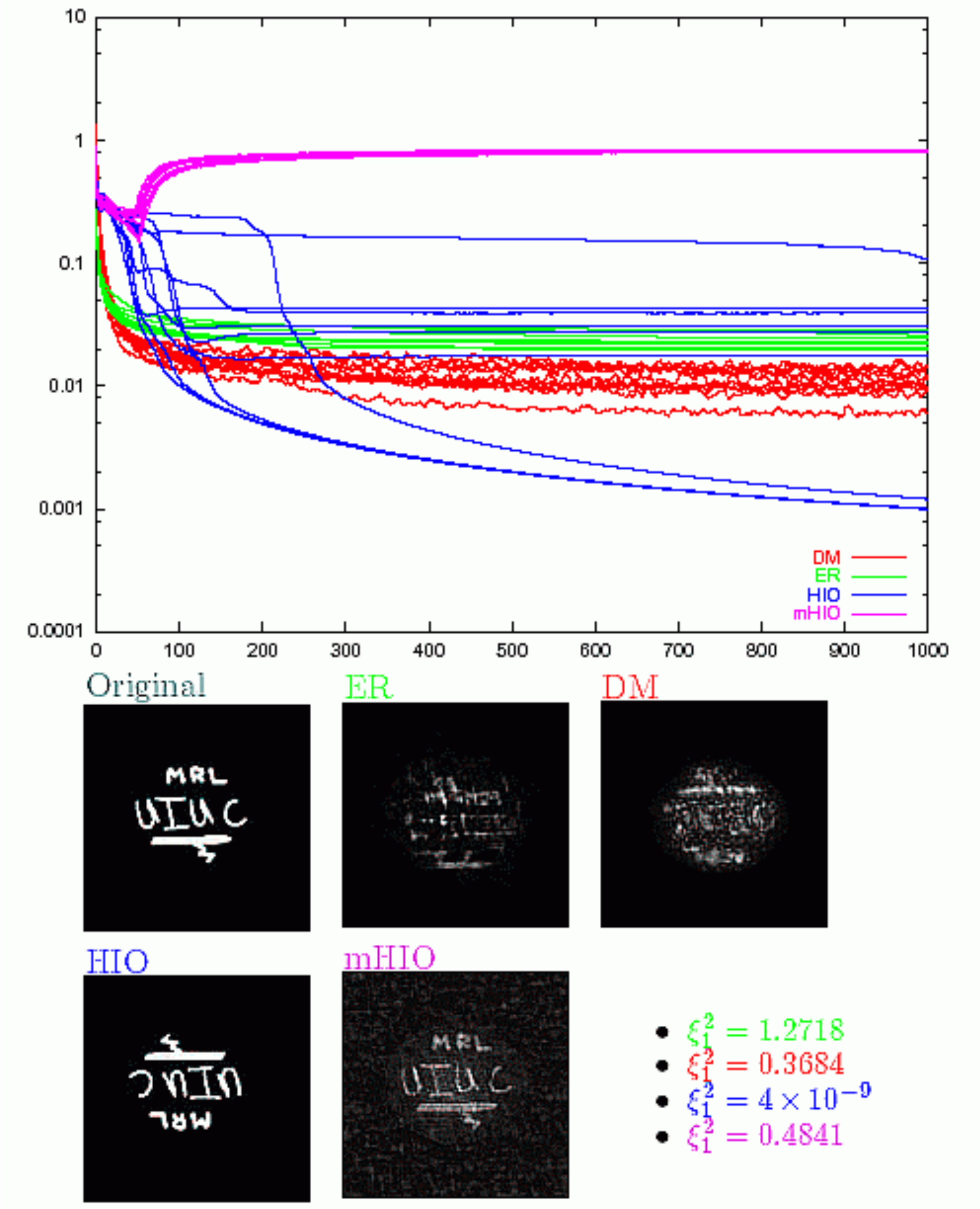




Label	Algorithm	Start x	Start y	Iterations	β	γ_1	γ_2
ER	ER	125	250	50	–	–	–
DM1	DM	125	250	50	0.7	-1	3.33
DM2	DM	125	250	50	0.7	-1.43	1.43
HIO	DM	125	250	50	0.7	-1	1.43
DM3	DM	500	250	50	0.1	-10	10
DM4	DM	500	250	50	0.7	-1	3.33

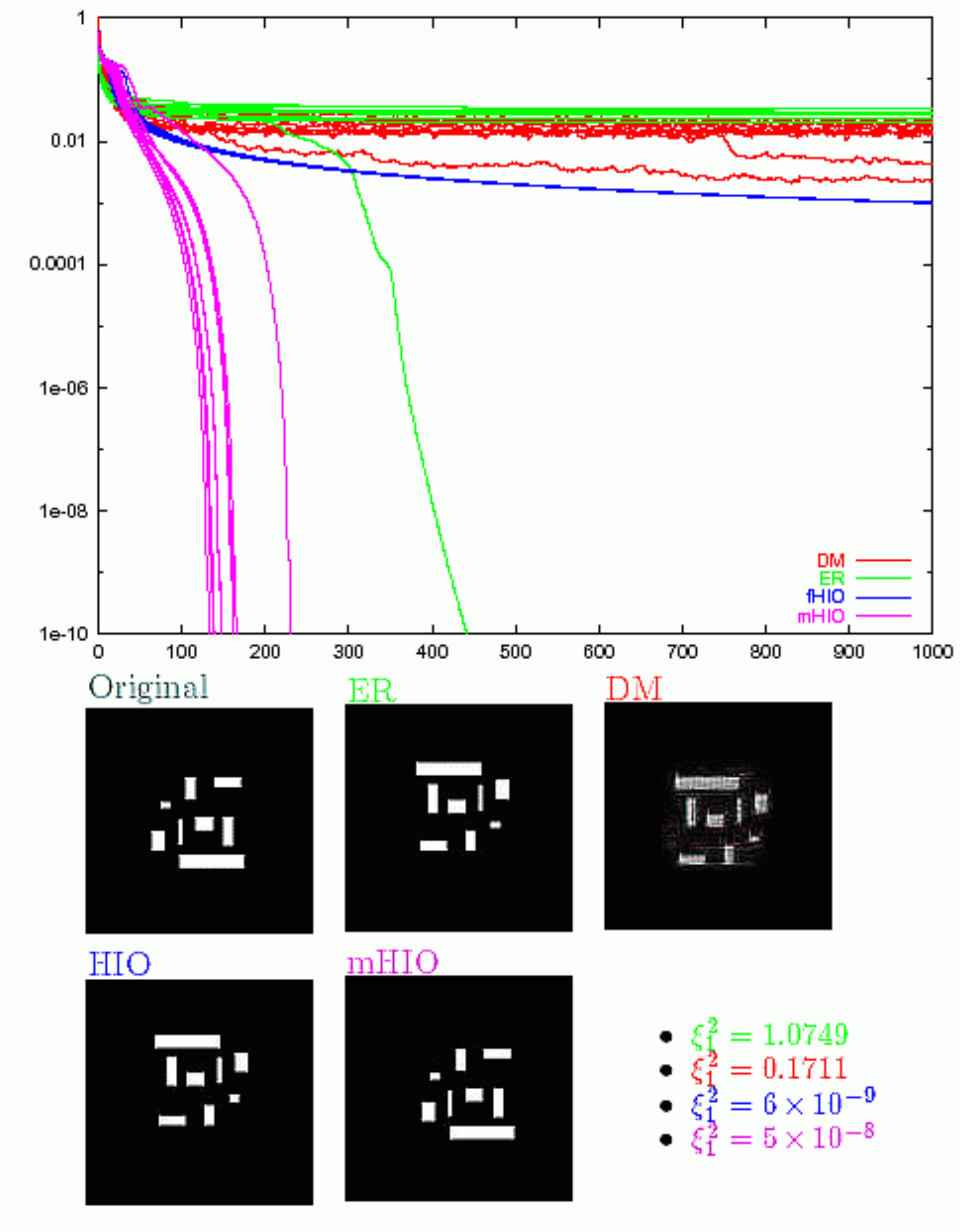
Label	Algorithm	Start x	Start y	Iterations	β	γ_1	γ_2
ER	ER	50	20	50	–	–	–
HIO1	DM	50	20	50	0.2	-1	5
DM1	DM	50	20	50	0.2	-5	5
DM2	DM	50	20	50	0.2	-10	10
HIO2	DM	50	20	50	1.2	-1	0.833
DM3	DM	50	20	50	1.2	-0.833	0.833
DM4	DM	50	20	50	-2	0.5	-1

Chapitre 4 de Garth Williams

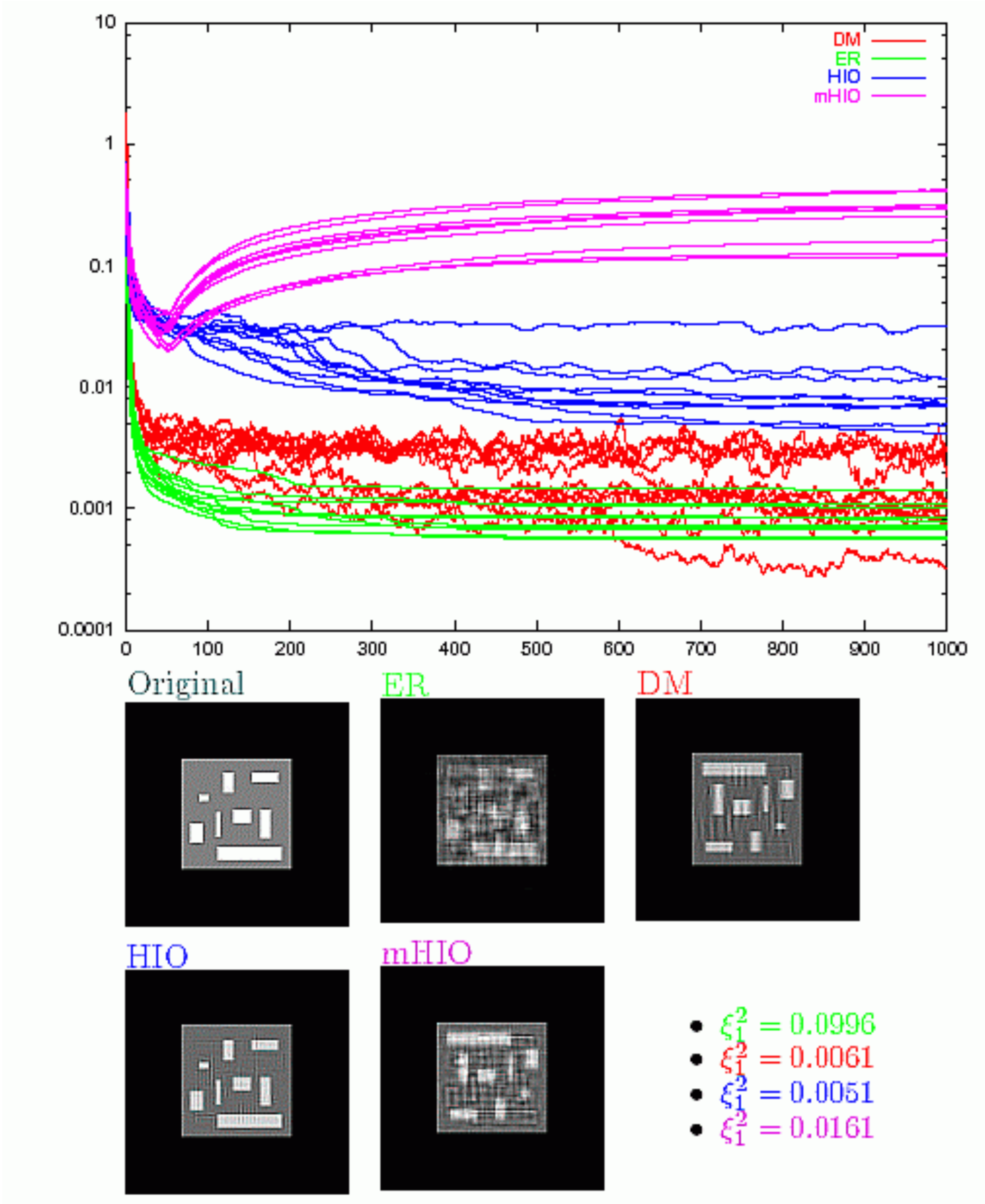


- $\xi_1^2 = 1.2718$
- $\xi_1^2 = 0.3684$
- $\xi_1^2 = 4 \times 10^{-9}$
- $\xi_1^2 = 0.4841$

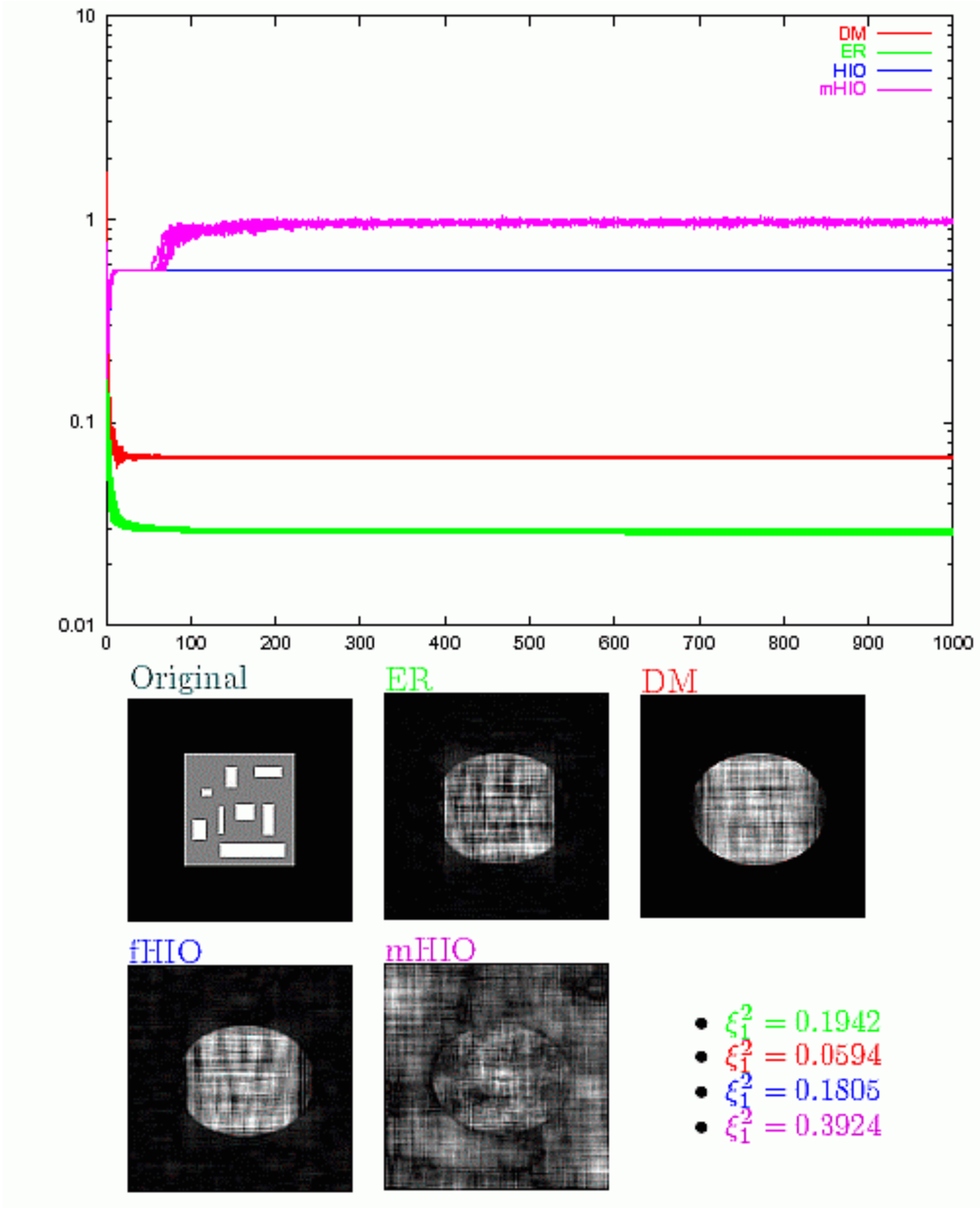
Convergence: écriture



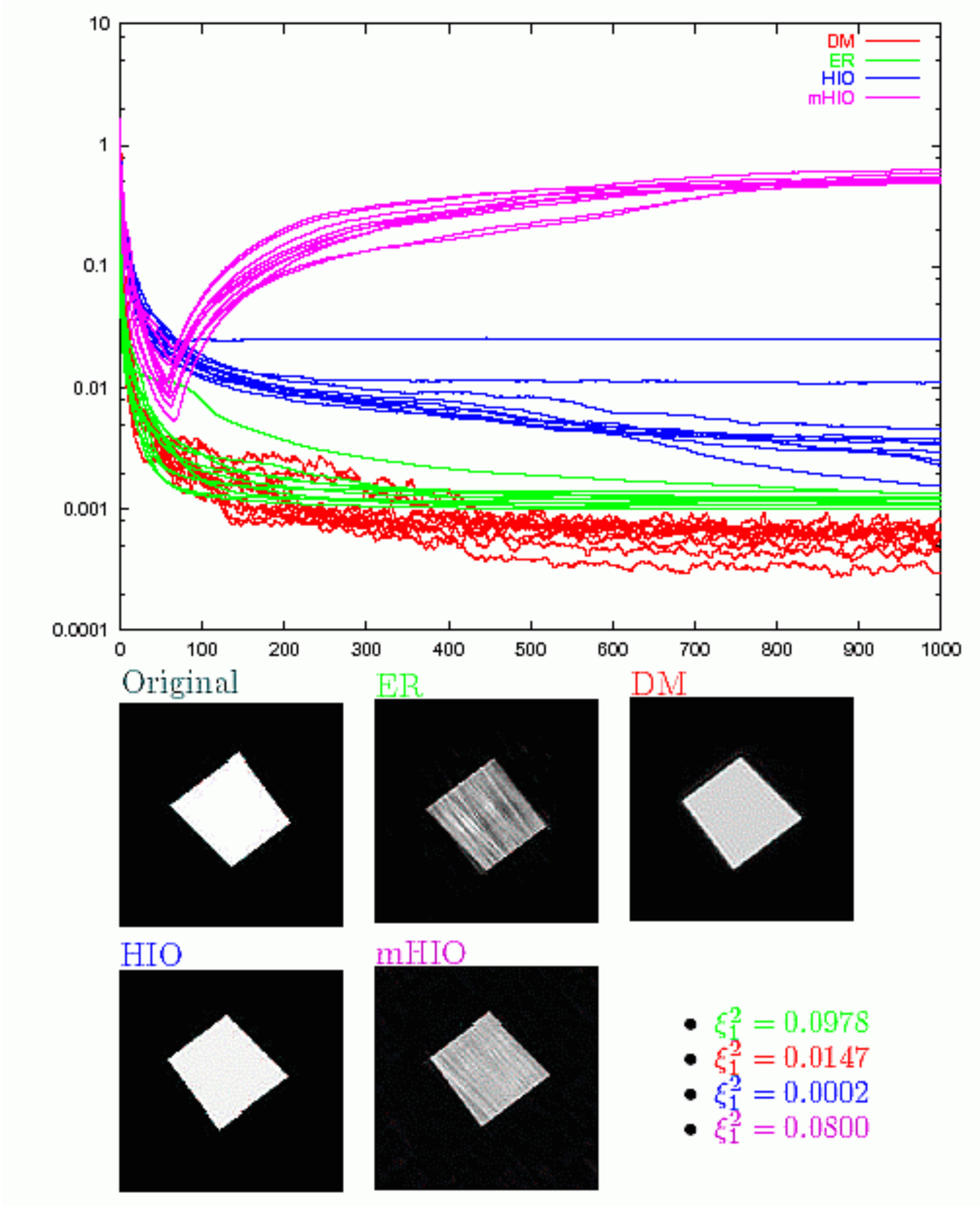
Convergence: rectangles



Convergence: rectangles (échelle grise)

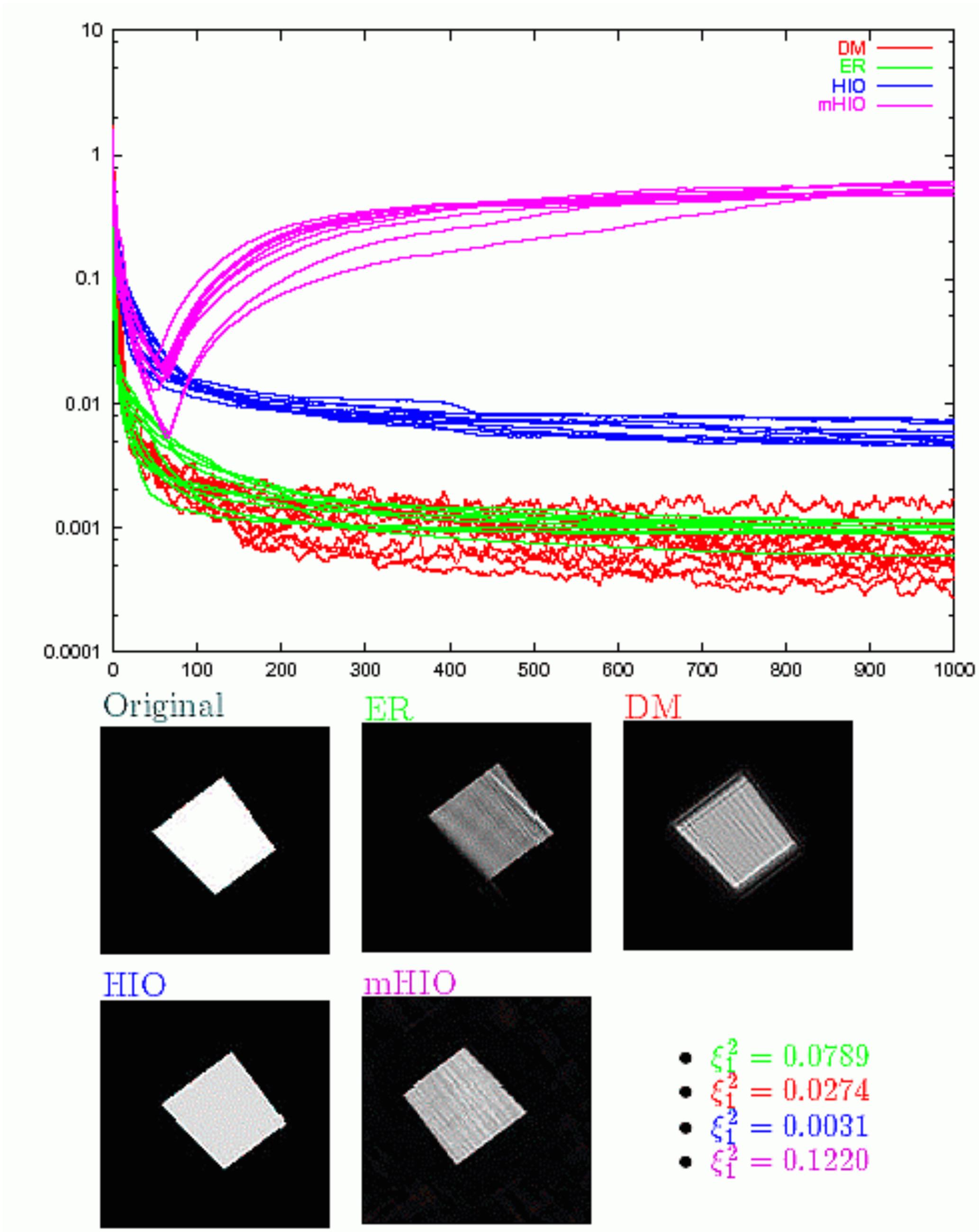


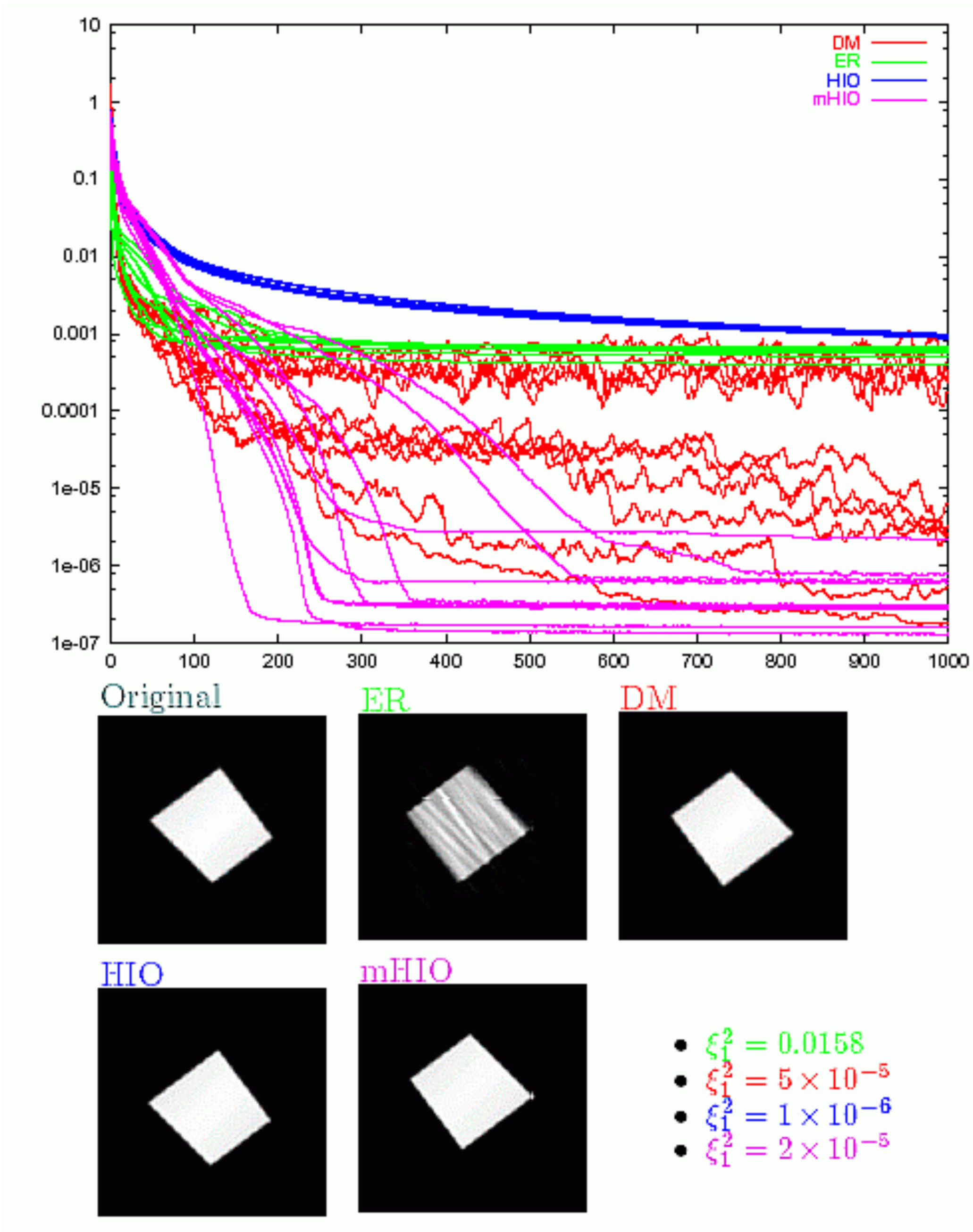
Convergence: rectangles (échelle grise) Support est trop petit



Convergence: polygone

Convergence: polygone Support Oval





Convergence: polygone Bords rugueux

Reconstruction imparfait peut être rayé

0.5 micron Pb cristal sur SiO_2 substrate

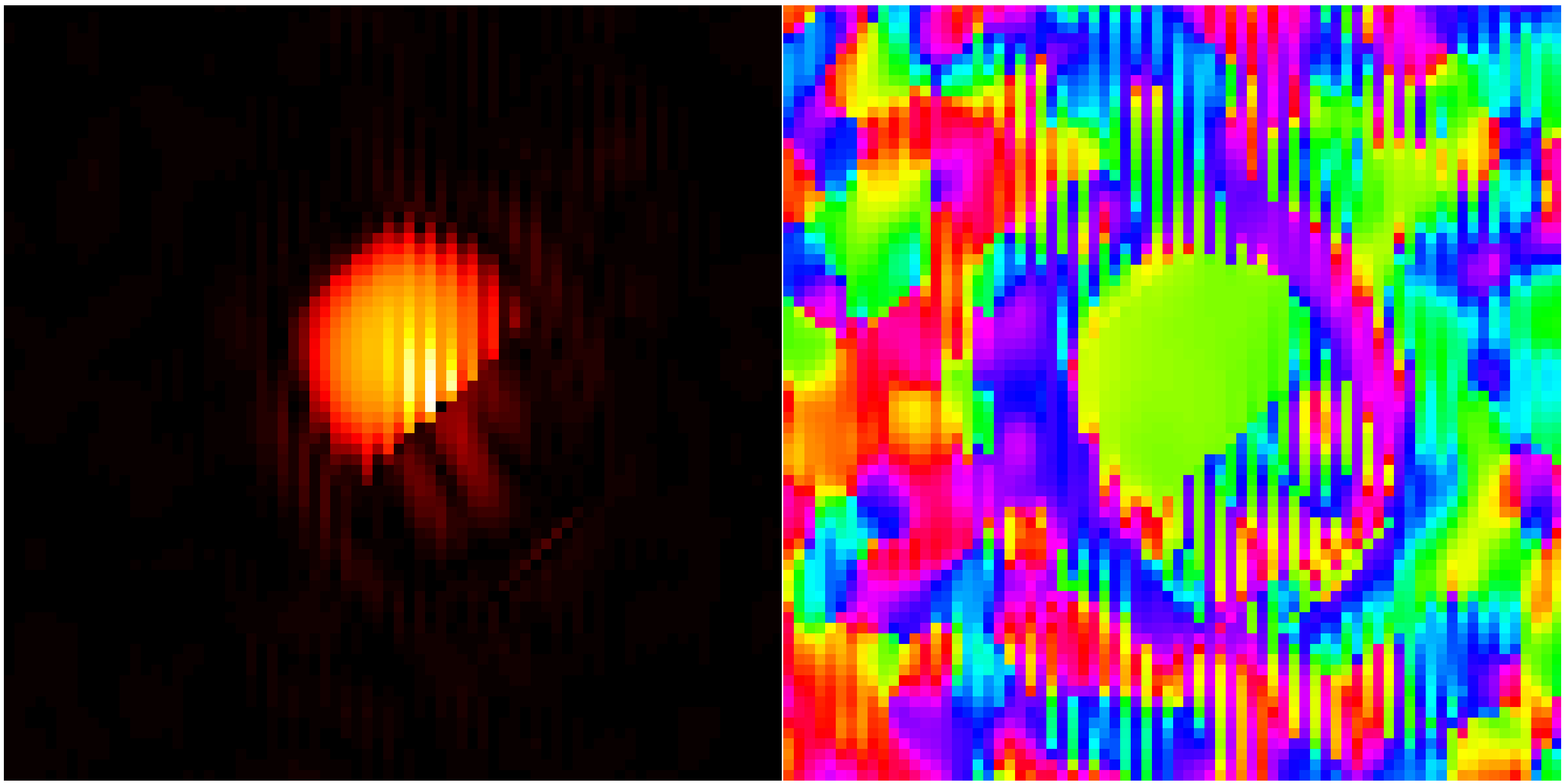
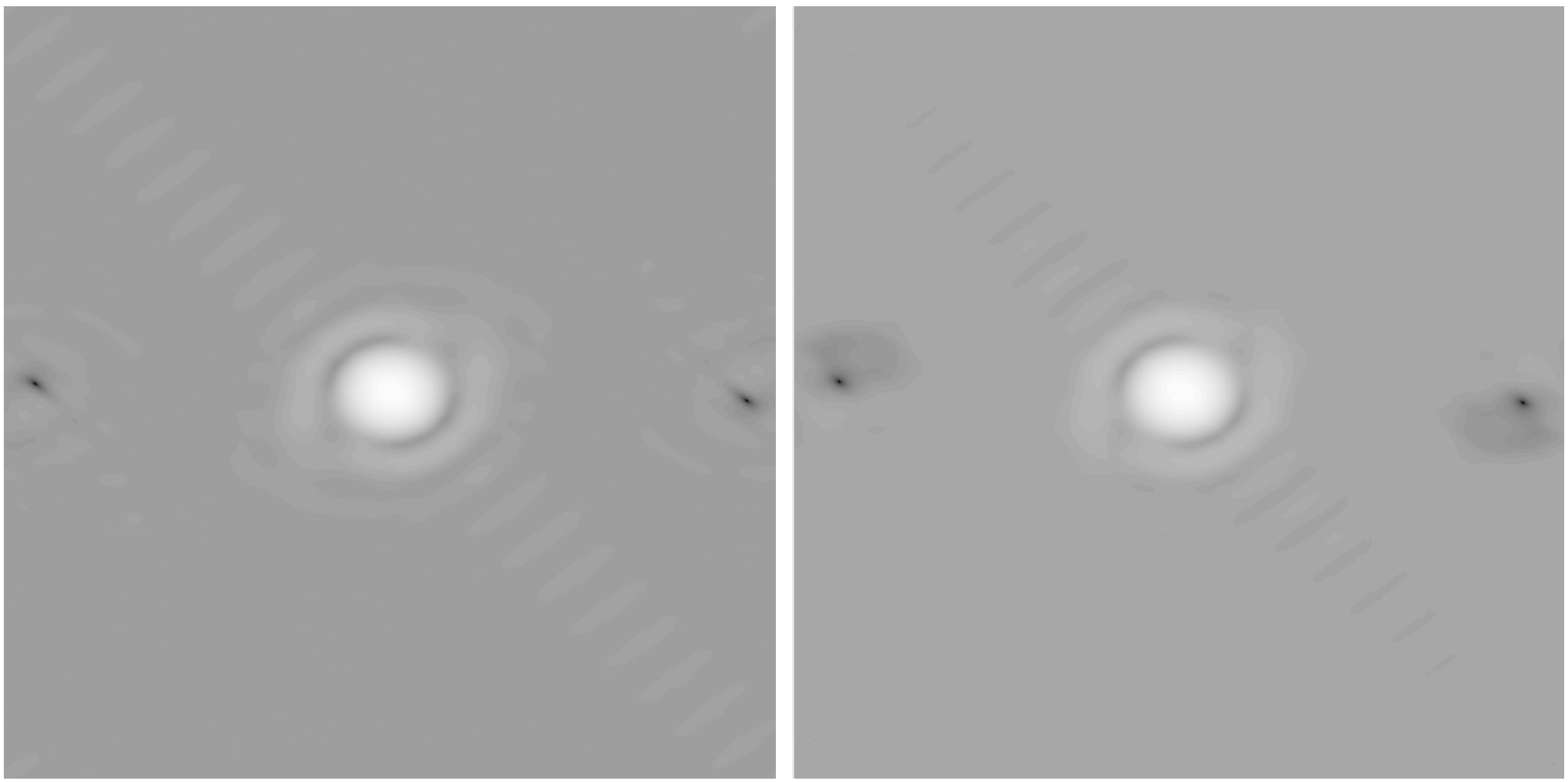


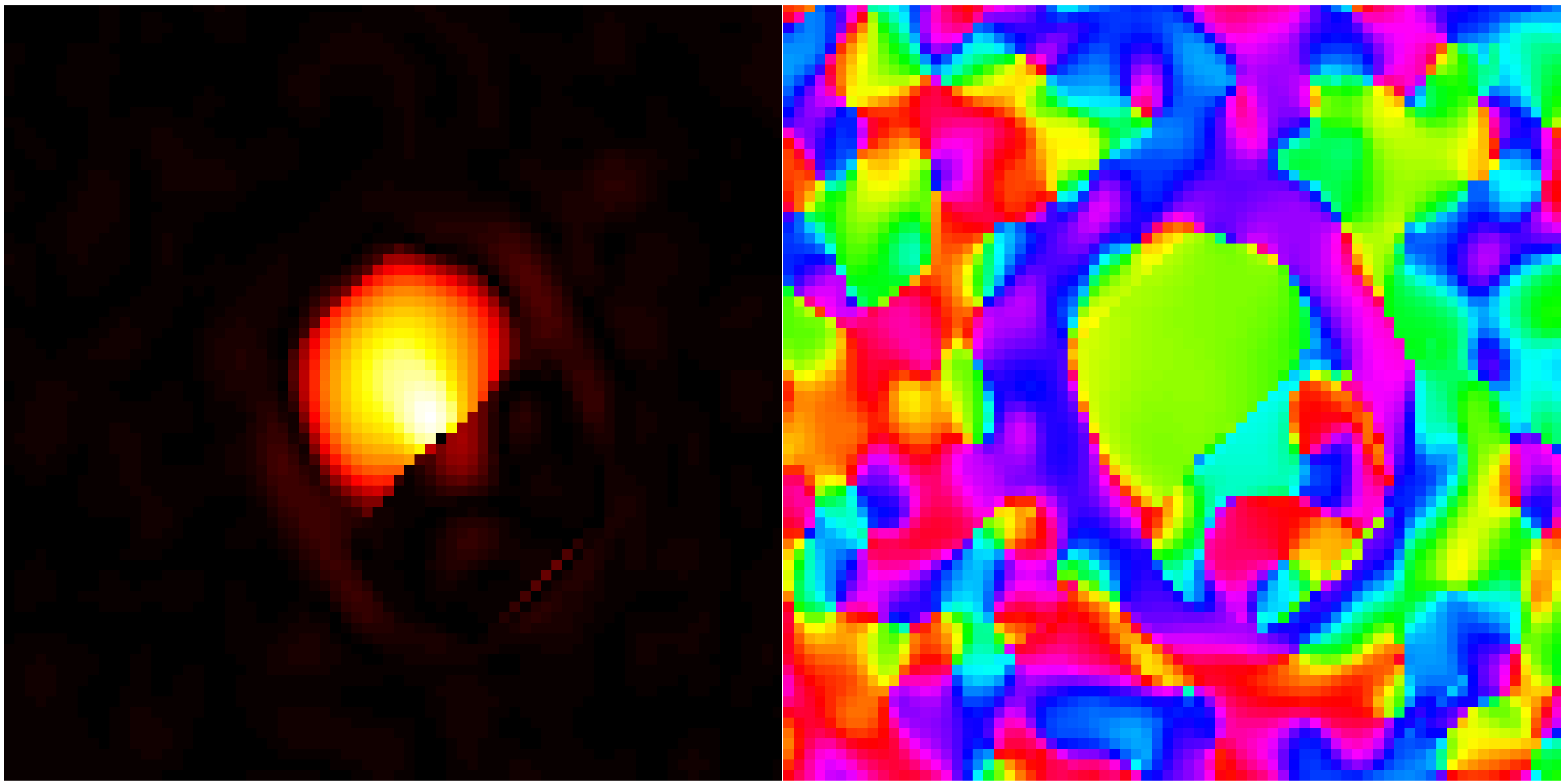
Image rayé attribué aux “Vortices”

Vortex pairs separated by inverse of stripe spacing

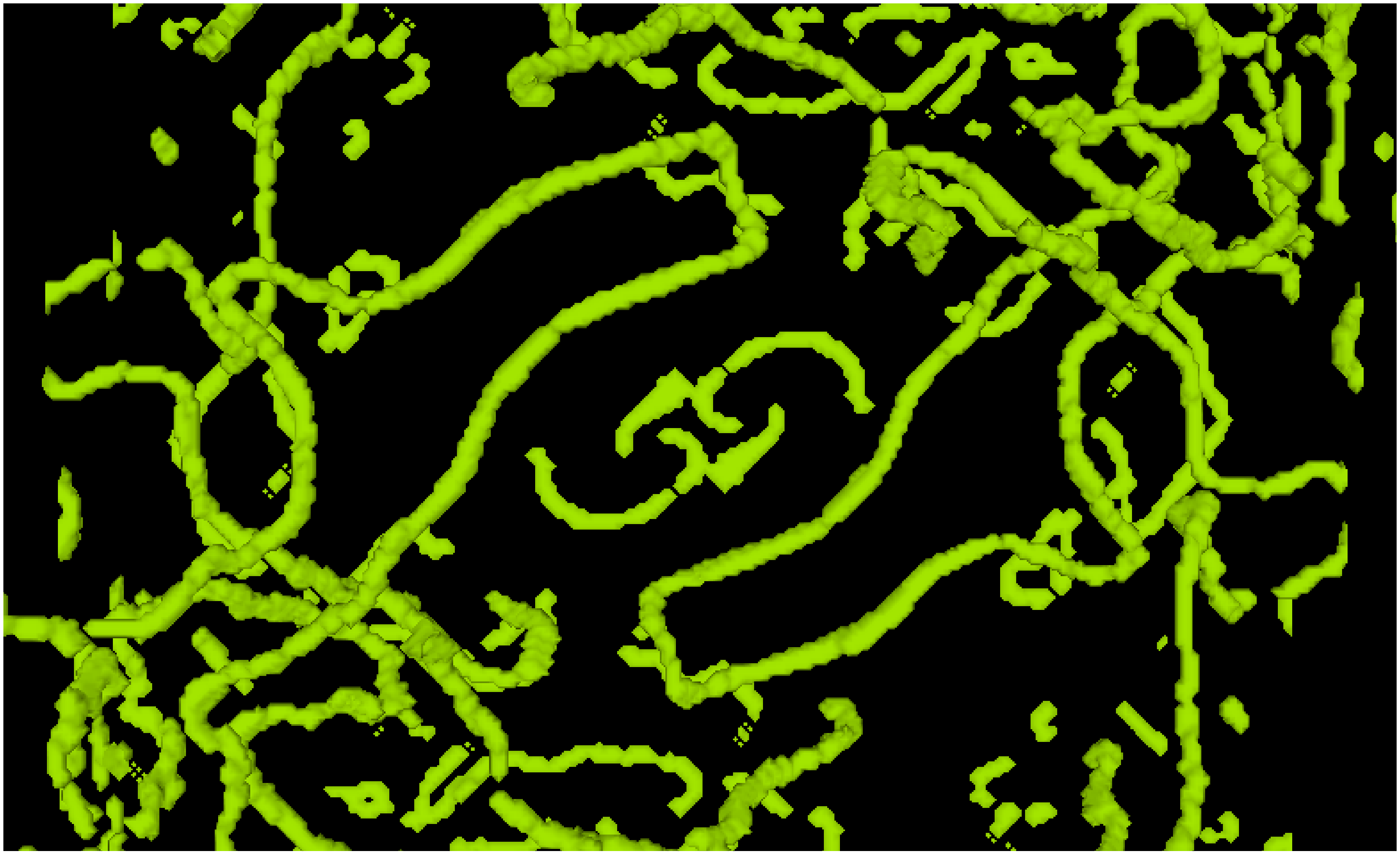


Result of “Patching” in 2D

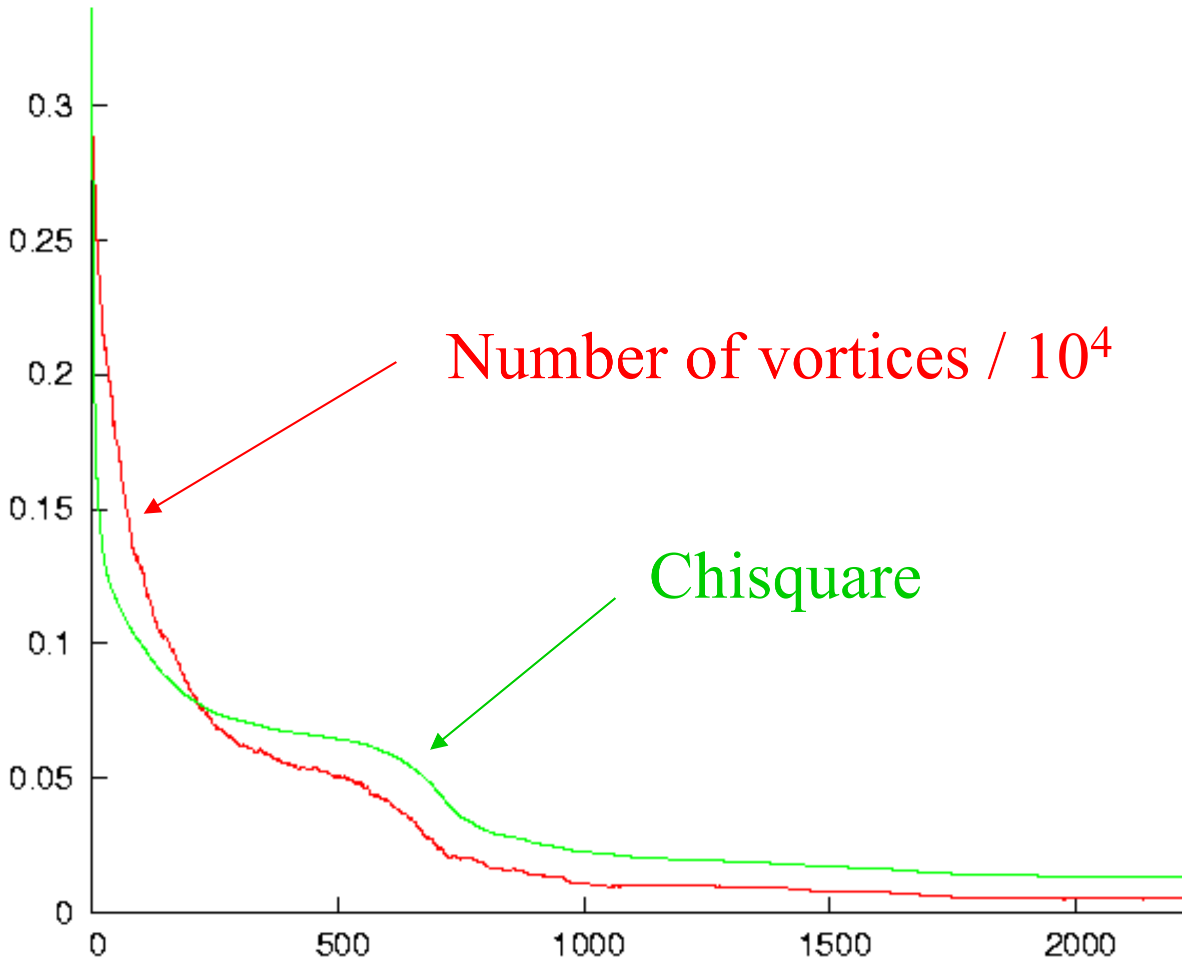
J. R. Fienup Appl. Opt. 21 2758 (1982)



3D Vortices Form Pairs of Loops



Vortices are a Cause of Stagnation during Error Reduction



Sommaire

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- Thèse de Garth Williams:
  - https://netfiles.uiuc.edu/gjwillms/shared/thesis.pdf