

# Algorithmes pour rechercher la phase des diagrammes de diffraction cohérentes

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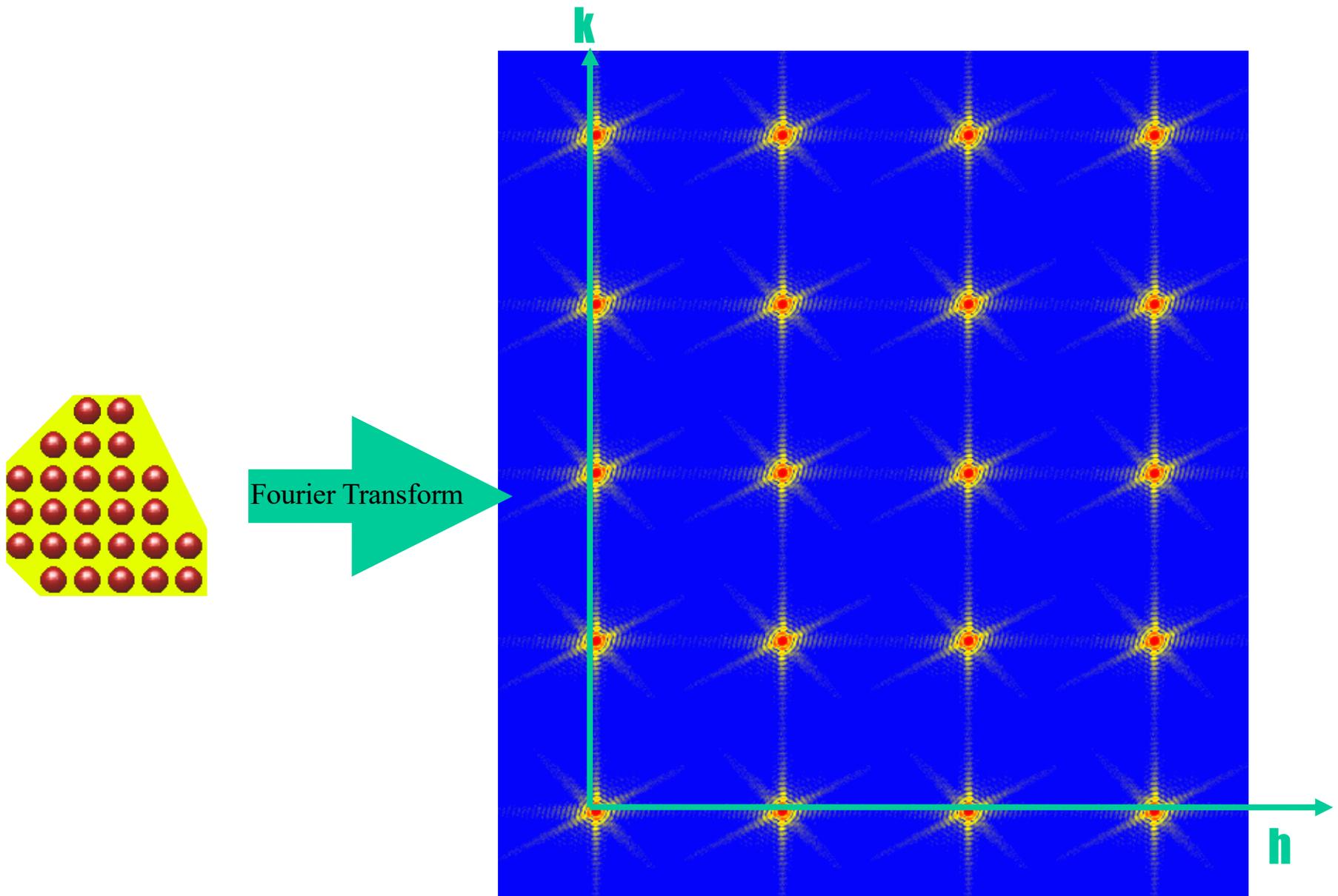
Department of Physics  
University of Illinois

Journée Scientifique sur  
Diffraction et Diffusion  
des X Coherents  
Grenoble, Octobre 2004

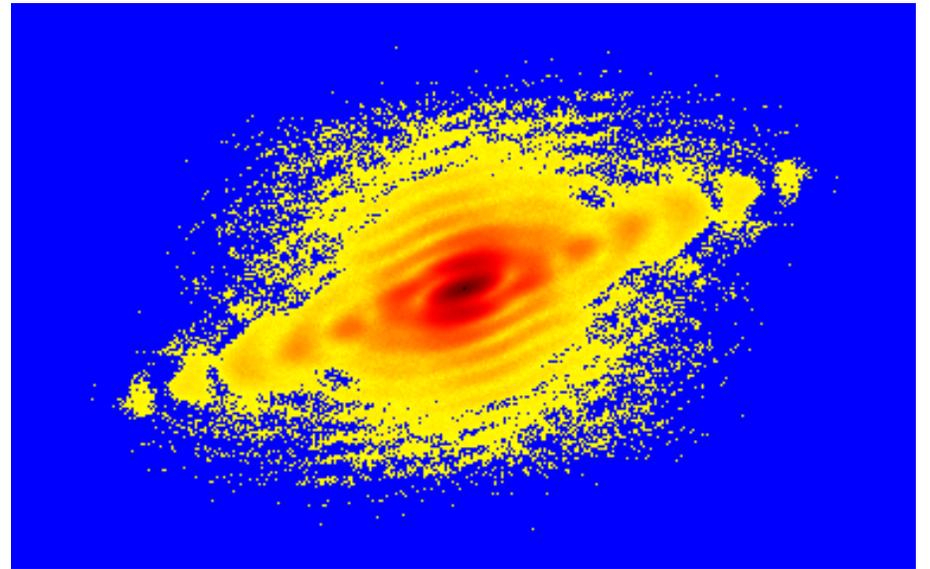
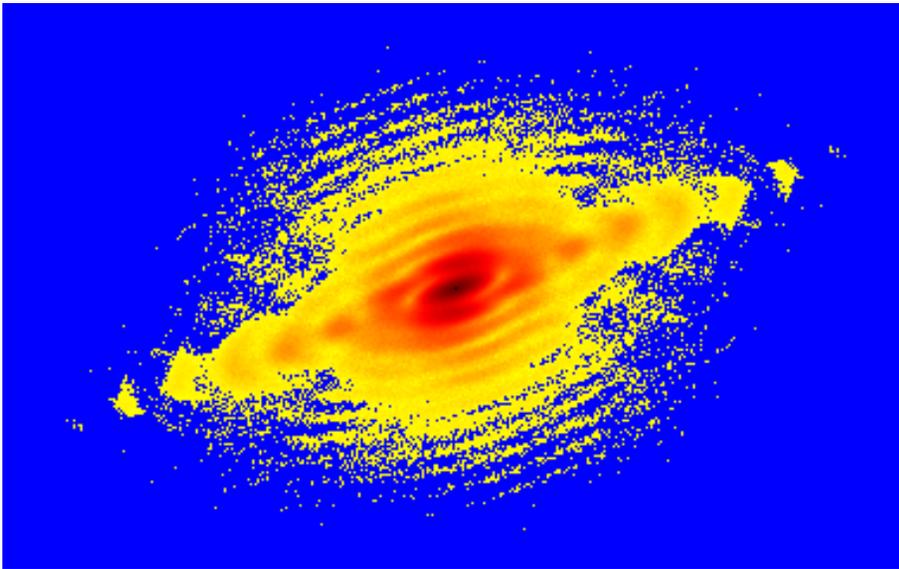
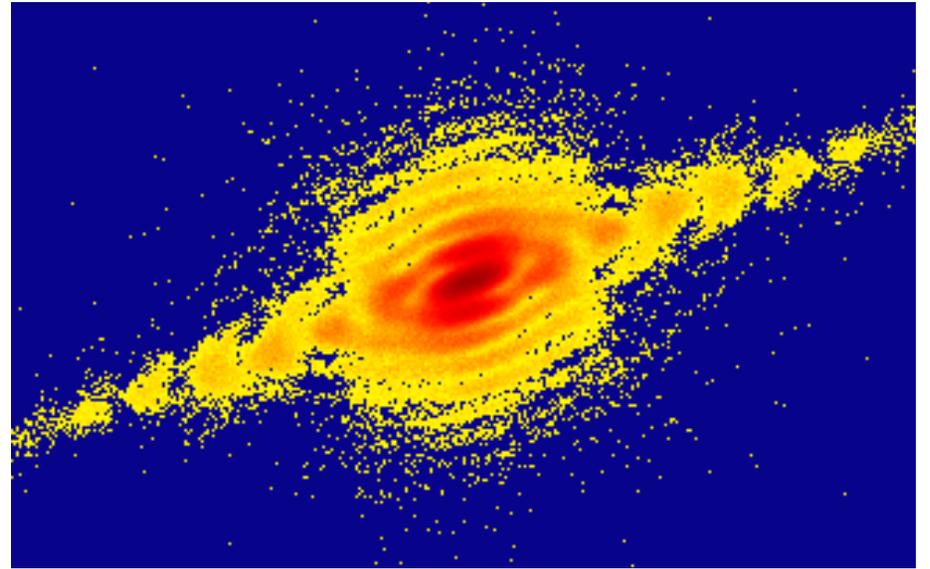
# Resumé

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

# Diffusion cohérente des Cristaux

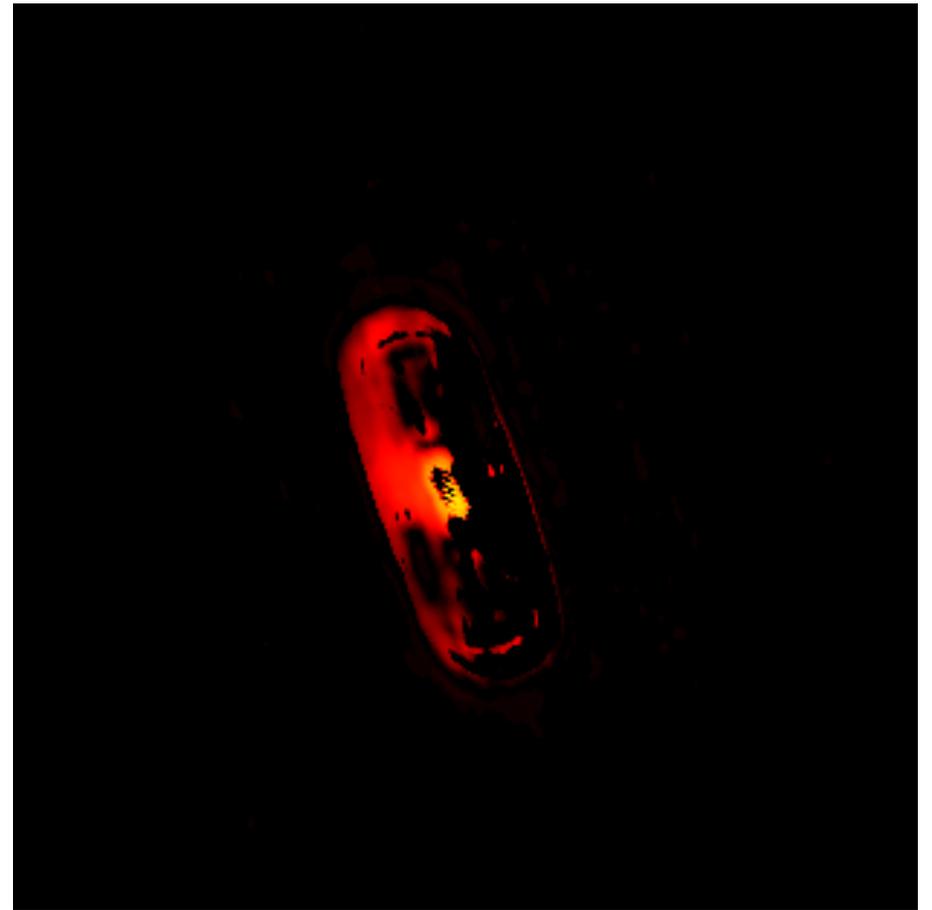
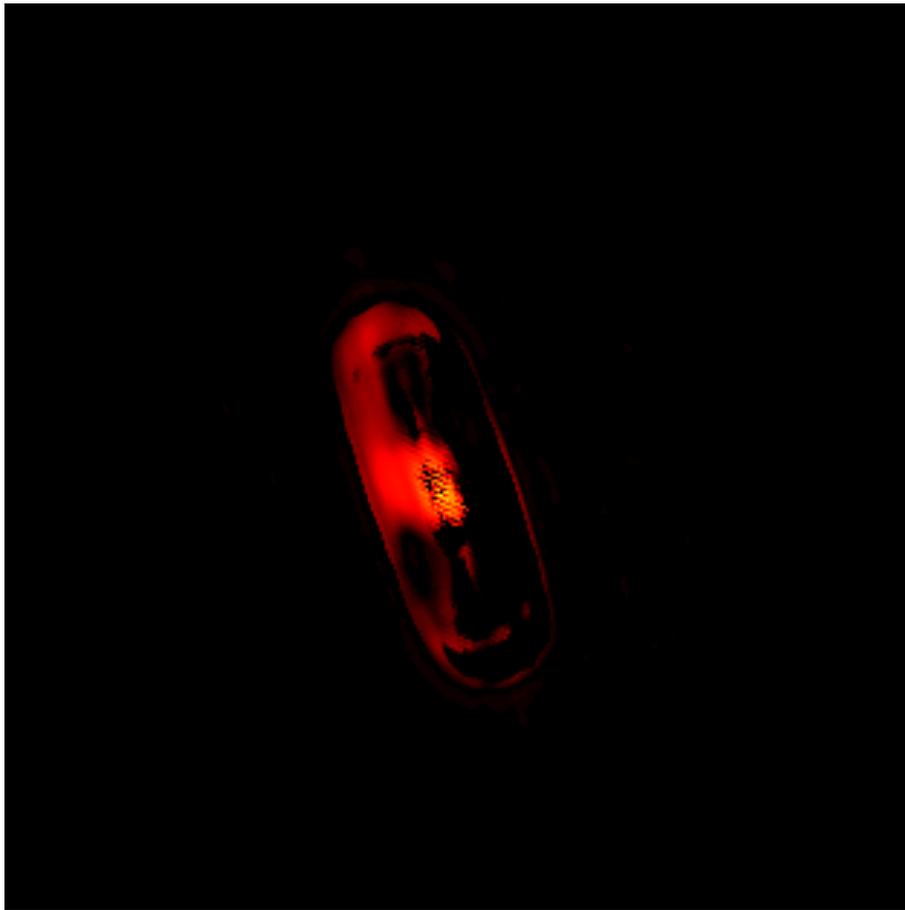


Données CCD et  
Ajustements  
 $\text{Chisq}=0.0005$

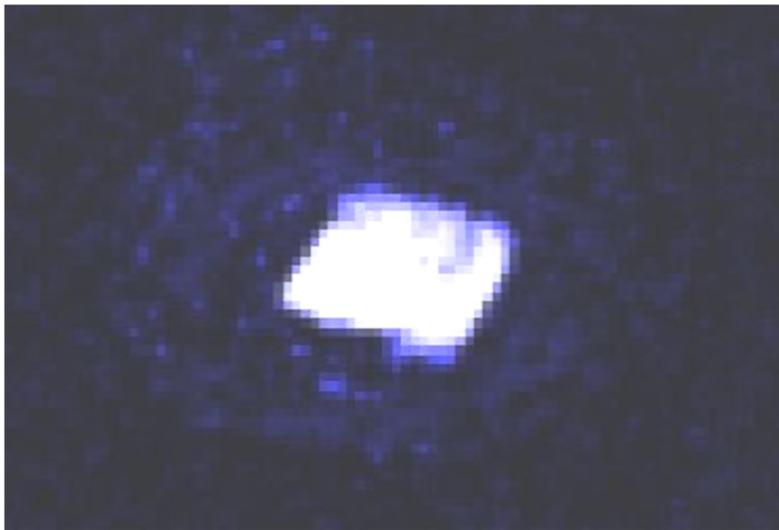


# 2D Reconstructions

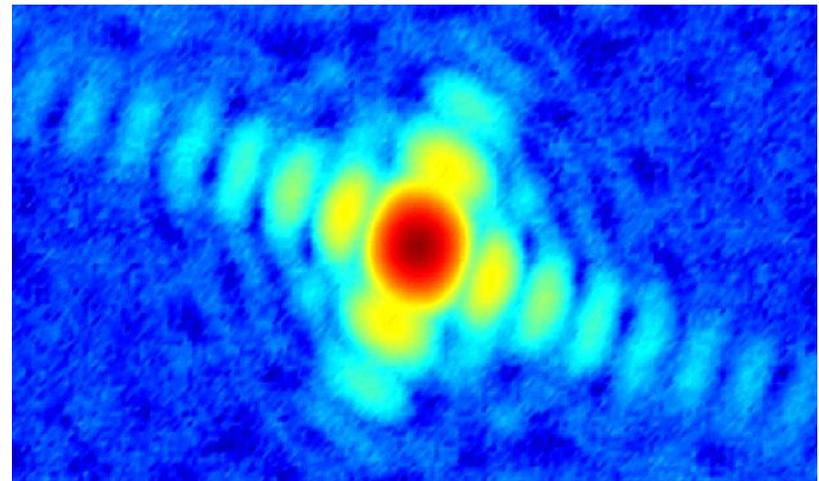
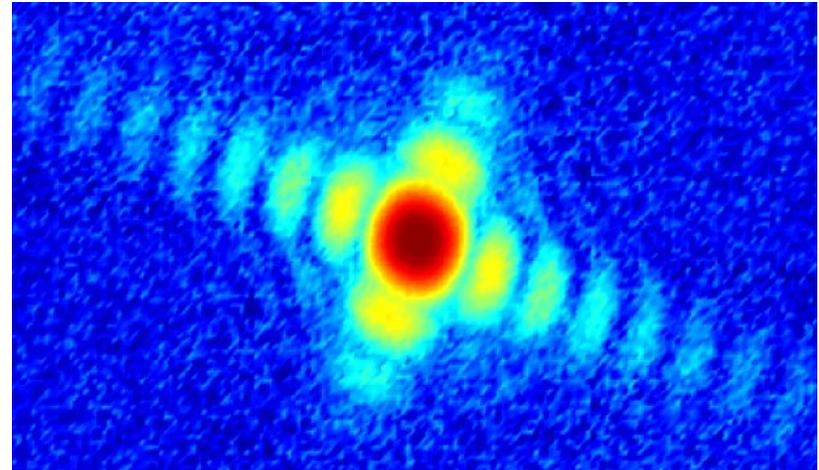
chisquare = 0.0005



# Reconstruction of Ag Nanocrystal



←→  
200nm



# Unicité (uniqueness) par Convolution

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

$$h(z) = f(z) \otimes g(z) \quad (1.37)$$

and we may compose a second function

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

l via Hadamard's product:

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

# Demonstration de Uniqueness

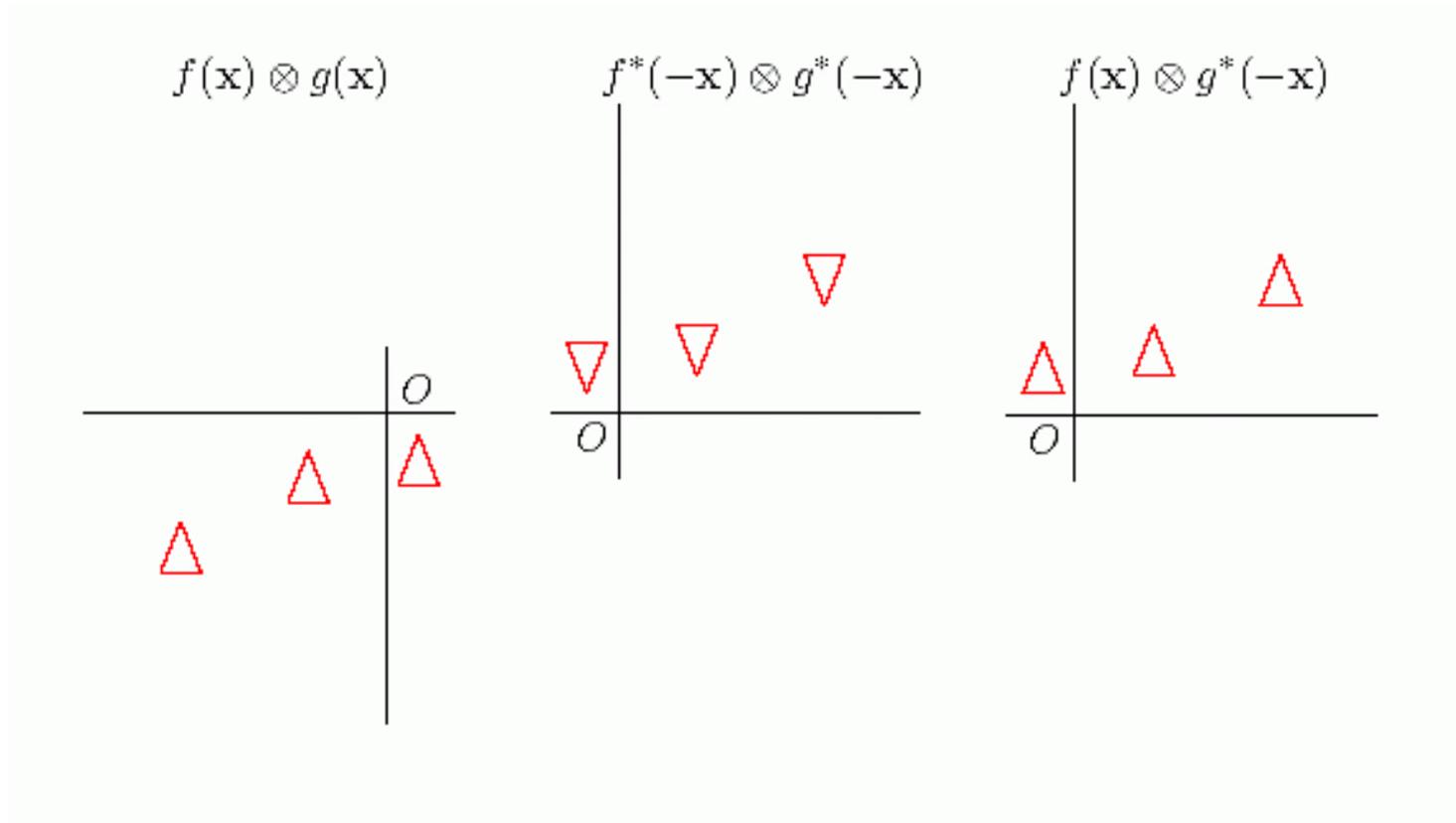
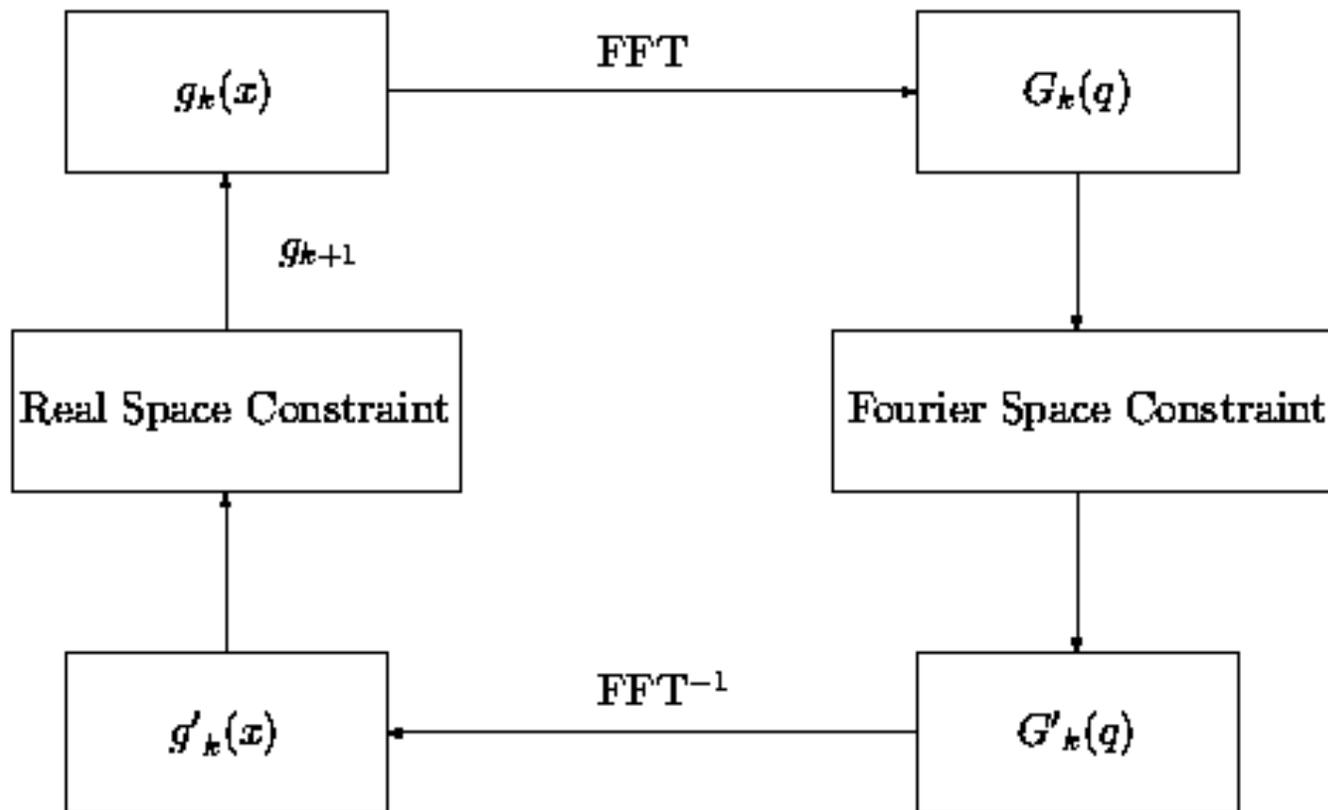


Figure 1.1: All three examples have the same Fourier magnitude, demonstrating that ambiguous solutions are possible in 2D.  $f(\mathbf{x})$  is the shape of the triangle.  $g(\mathbf{x}) = \delta(\mathbf{x} - \mathbf{x}_1) + \delta(\mathbf{x} - \mathbf{x}_2) + \delta(\mathbf{x} - \mathbf{x}_3)$ , where 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

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# Generic “Error Reduction” method



# Methode Gerchberg-Saxton (GS)

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

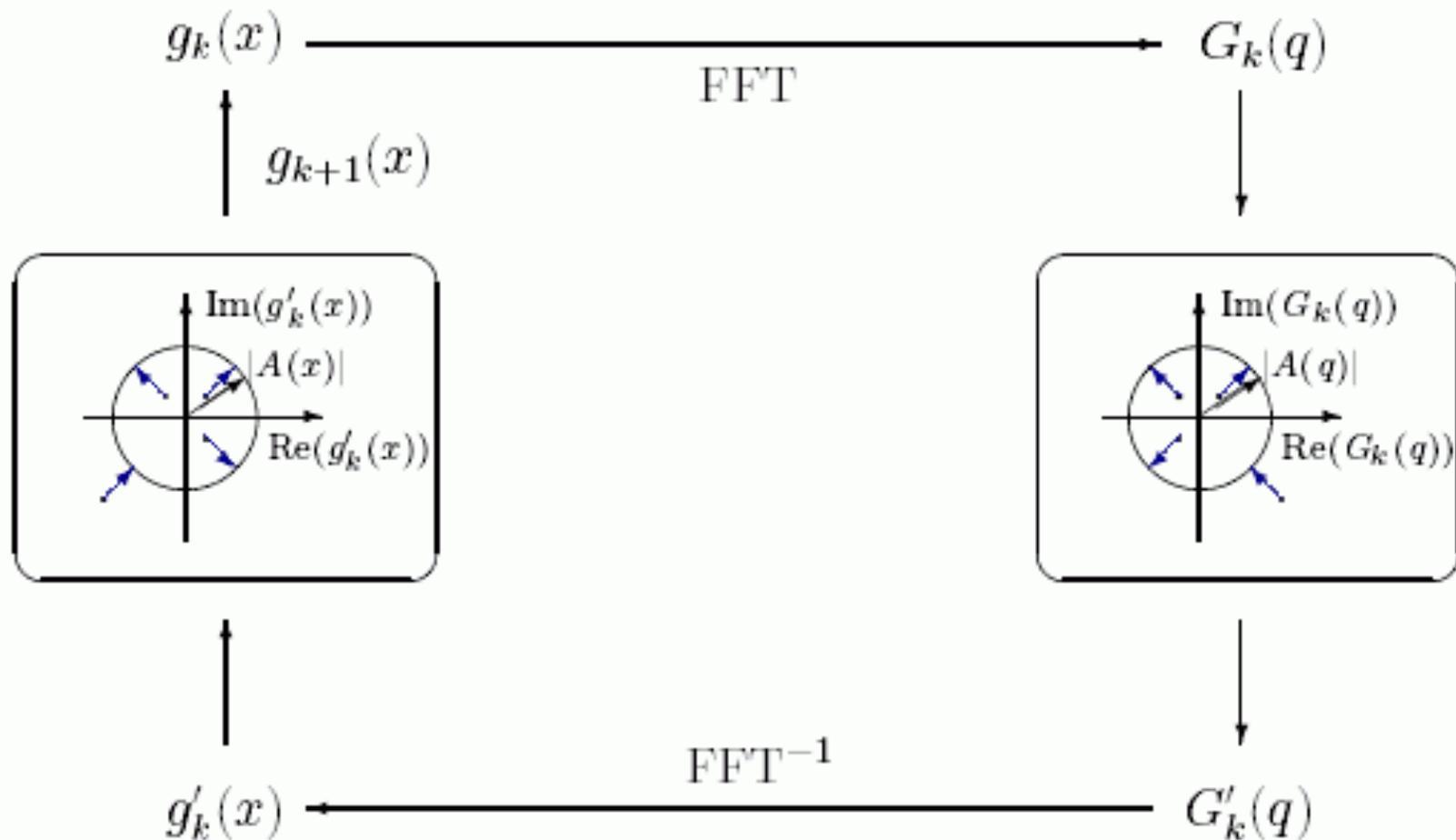


Figure 2.1: Gerchberg-Saxton Algorithm.

# Methode du Reduction d'Erreur (ER)

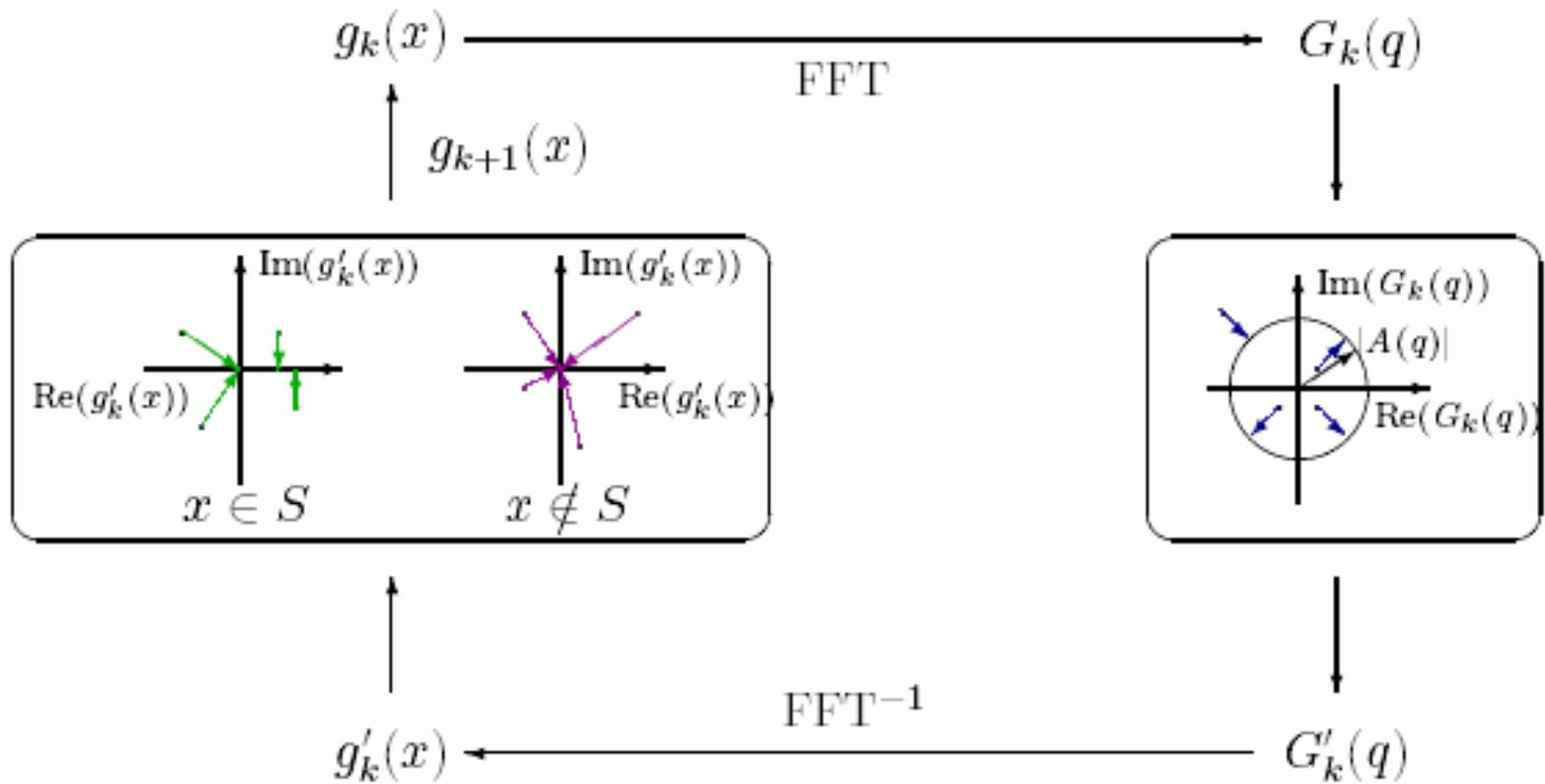


Figure 2.2: Error Reduction Algorithm.

# Methode HIO de Fienup

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

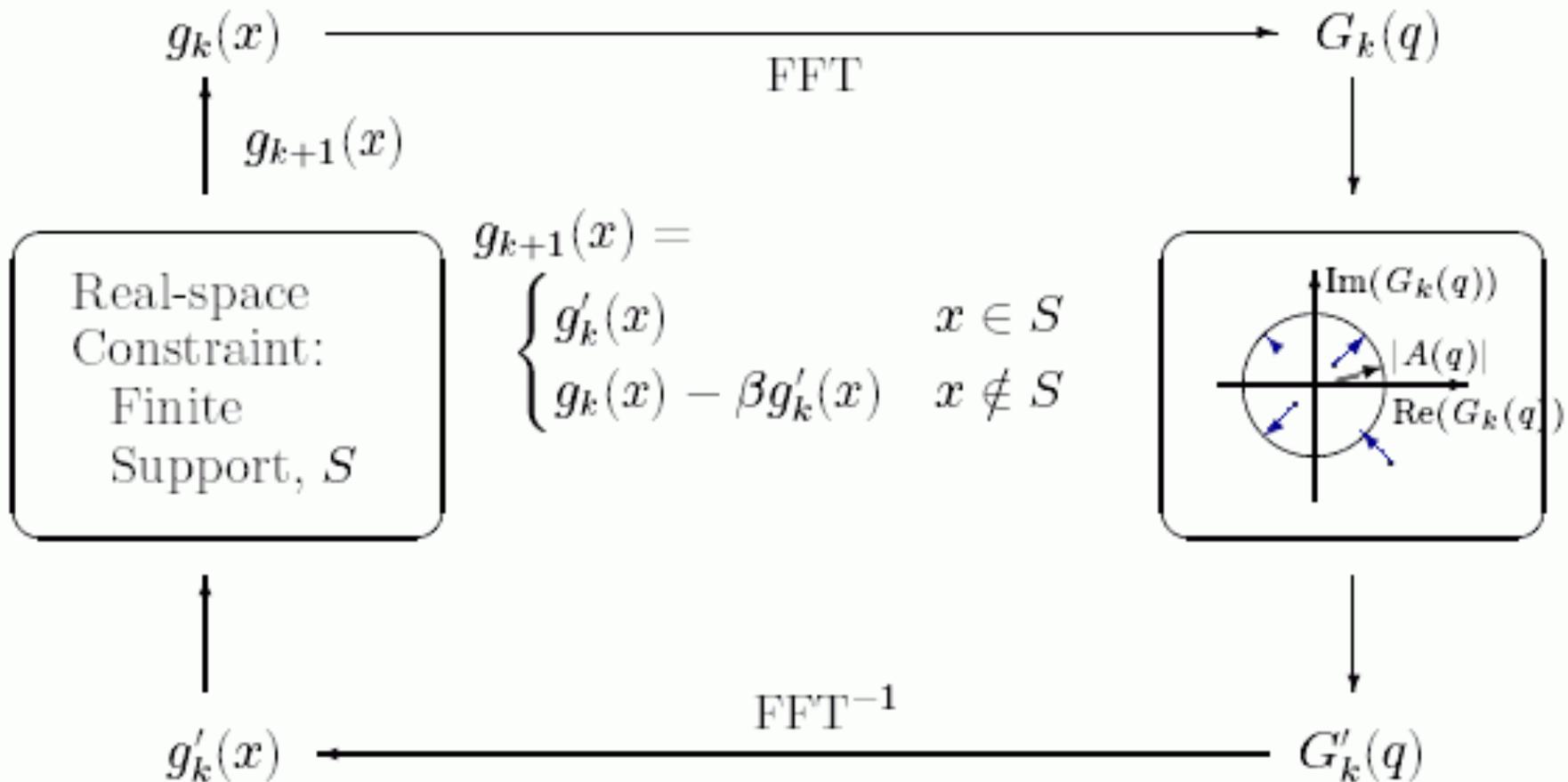


Figure 2.3: Fienup HIO

# Version HIO de Millane

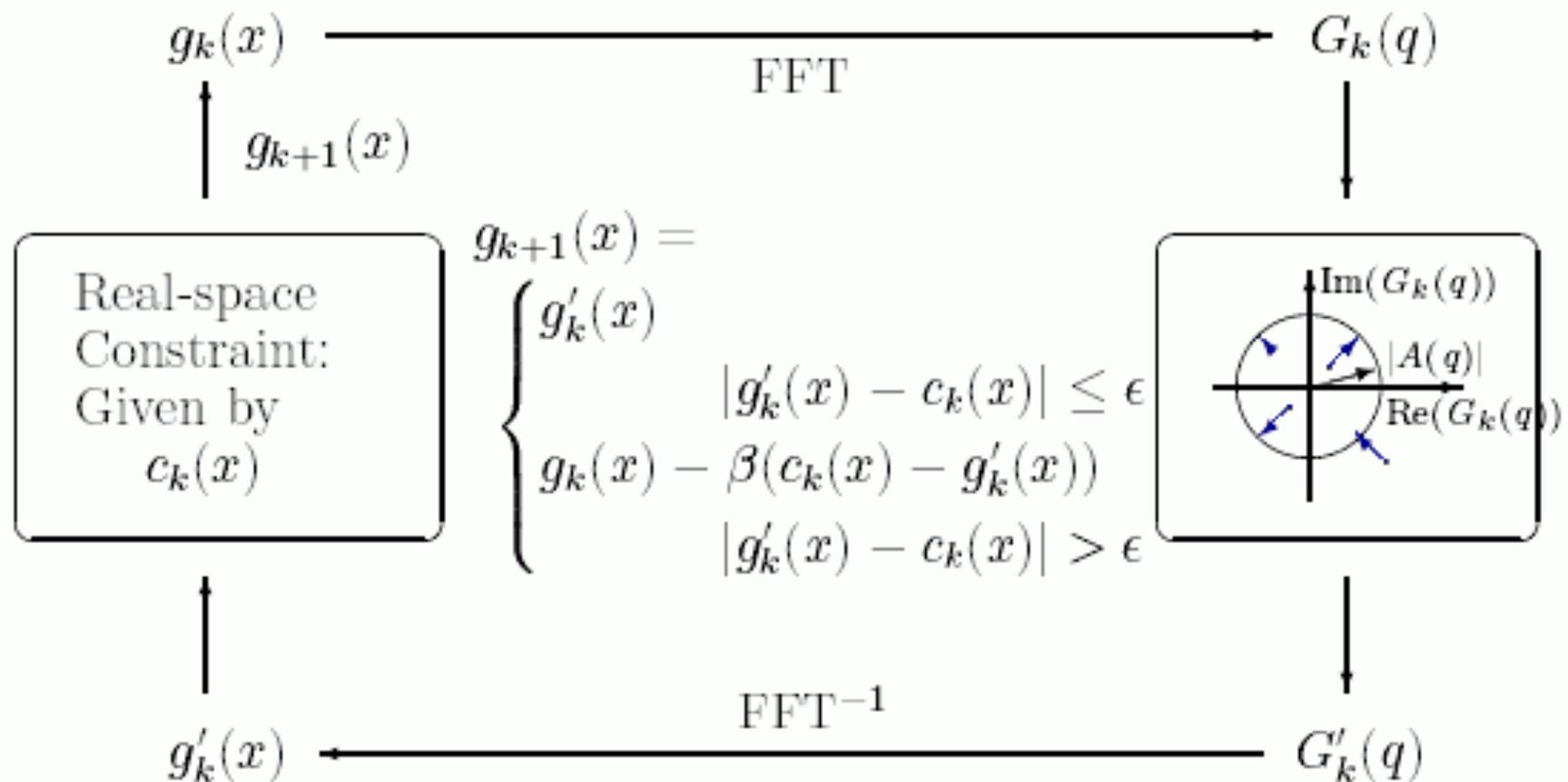


Figure 2.4: Millane's HIO.

# Variations de “Hybrid Input-Output”

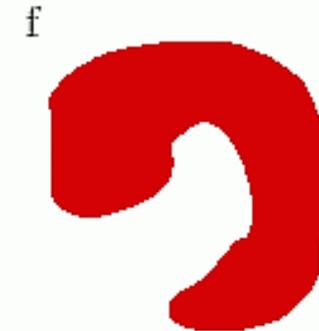
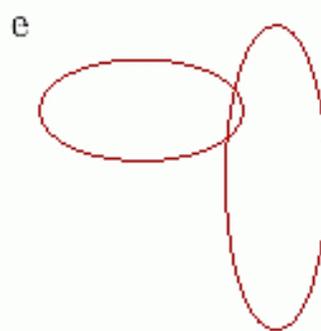
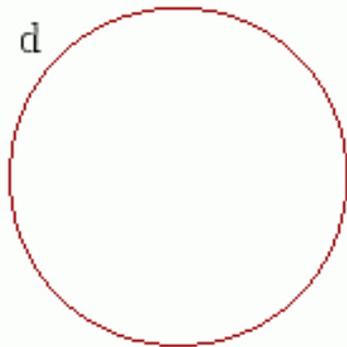
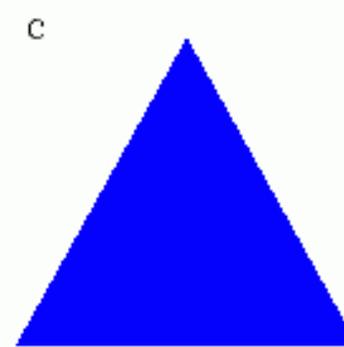
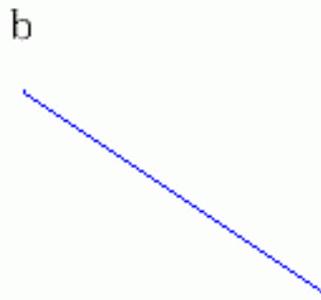
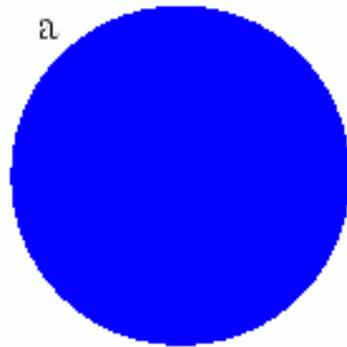
$$g_{k+1} = \begin{cases} g'_k & \text{if } x \in S \\ 0 & \text{if } x \notin S \end{cases}. \quad (2.7) \quad \text{Reduction d'erreur}$$

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

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

HIO Millane

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



Ensembles  
Convexes

Ensembles  
Non-convexes

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.

# Trajectoire de l'Algorithme ER

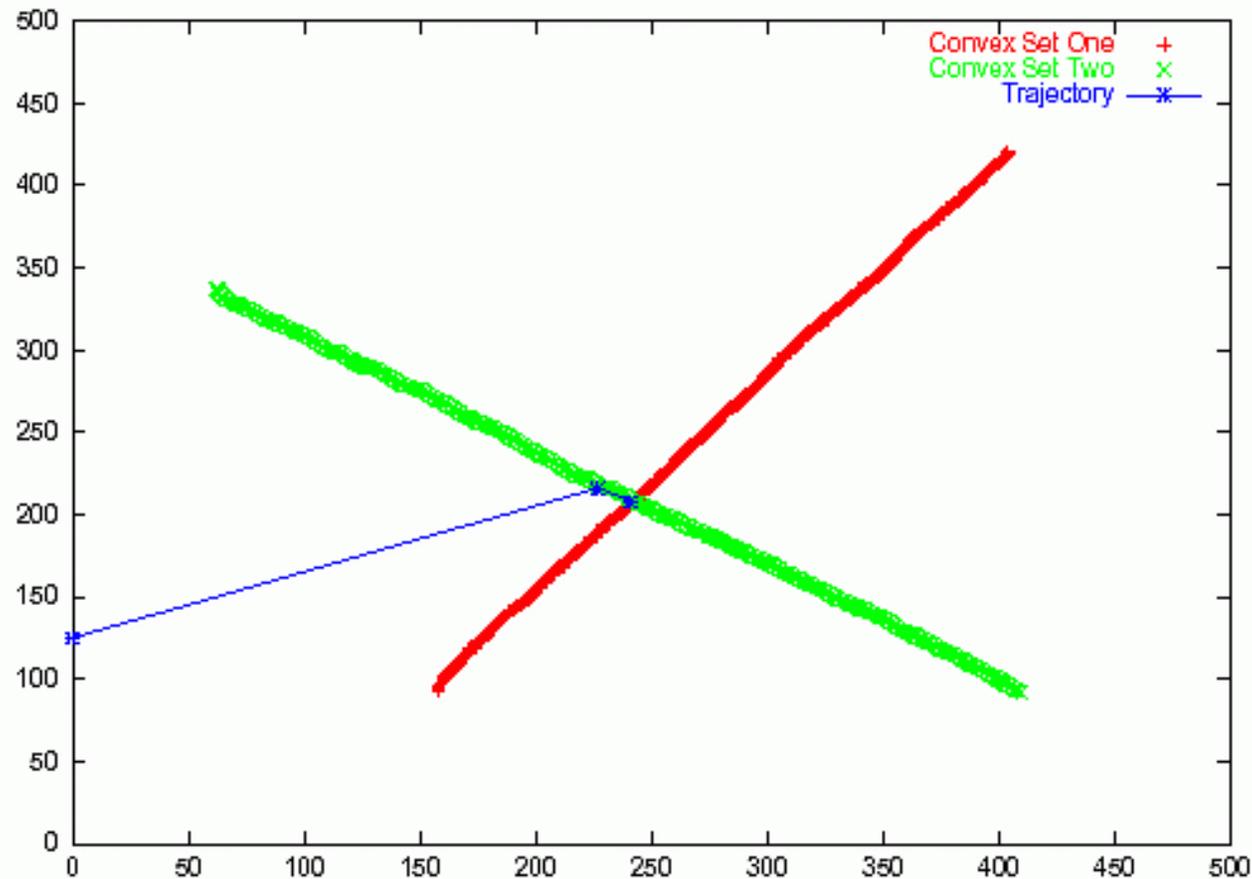


Figure 2.6: Trajectory of GS/ER. Because these two are alternating projection algorithms, the iterate will follow the contour of the boundary of a set.

# Trajectoire de l'Algorithme HIO

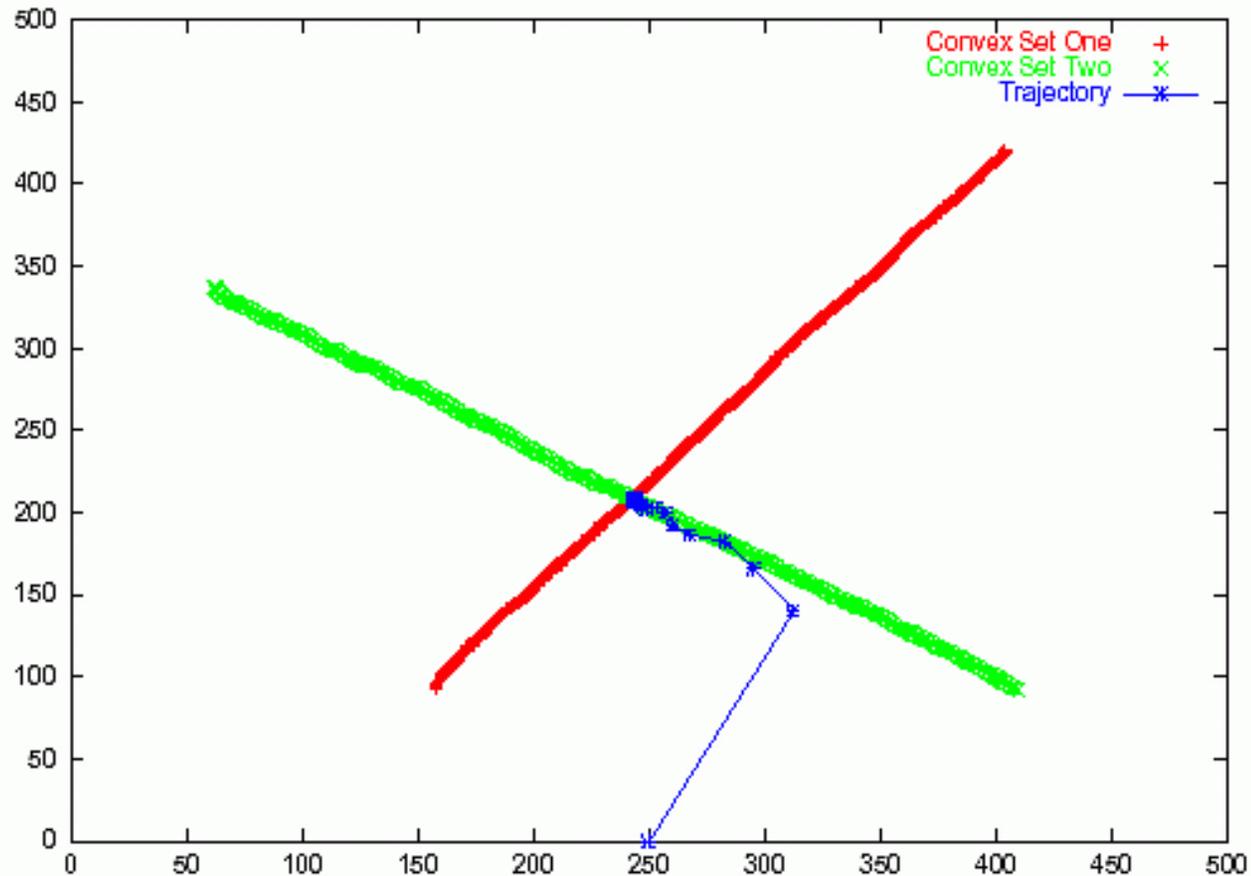


Figure 2.7: Trajectory of HIO. HIO does not follow the contour of the set as strictly as GS/ER. It has a tendency to spiral inward toward the intersection. For this example,  $\beta = 0.3$  has been chosen so that the step size is short and therefore better illustrates this behavior.

# Methode de Projections

$$\rho_{n+1} = (\pi_m(o)\pi_m(i))\rho_n. \quad (2.24)$$

Alg GS

$$\rho_{n+1} = (\pi_s\pi + \pi_m)\rho_n = (\pi_s + \pi_m)\rho_n, \quad (2.25)$$

Alg ER

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

Alg HIO

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

# Traitement de Veit Elser (Cornell): “Carte des Differences” = DM

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

$$f_i = (1 + \gamma_i)\pi_i - \gamma_i, \quad (2.30)$$

Mode I:  $\gamma_1 = -1$        $\gamma_2 = 1/\beta$       DM = HIO (Fienup)

Mode II:  $\gamma_1 = -1/\beta$        $\gamma_2 = 1/\beta$       “maximally contractive”

# Trajectoire de l'Algorithme DM

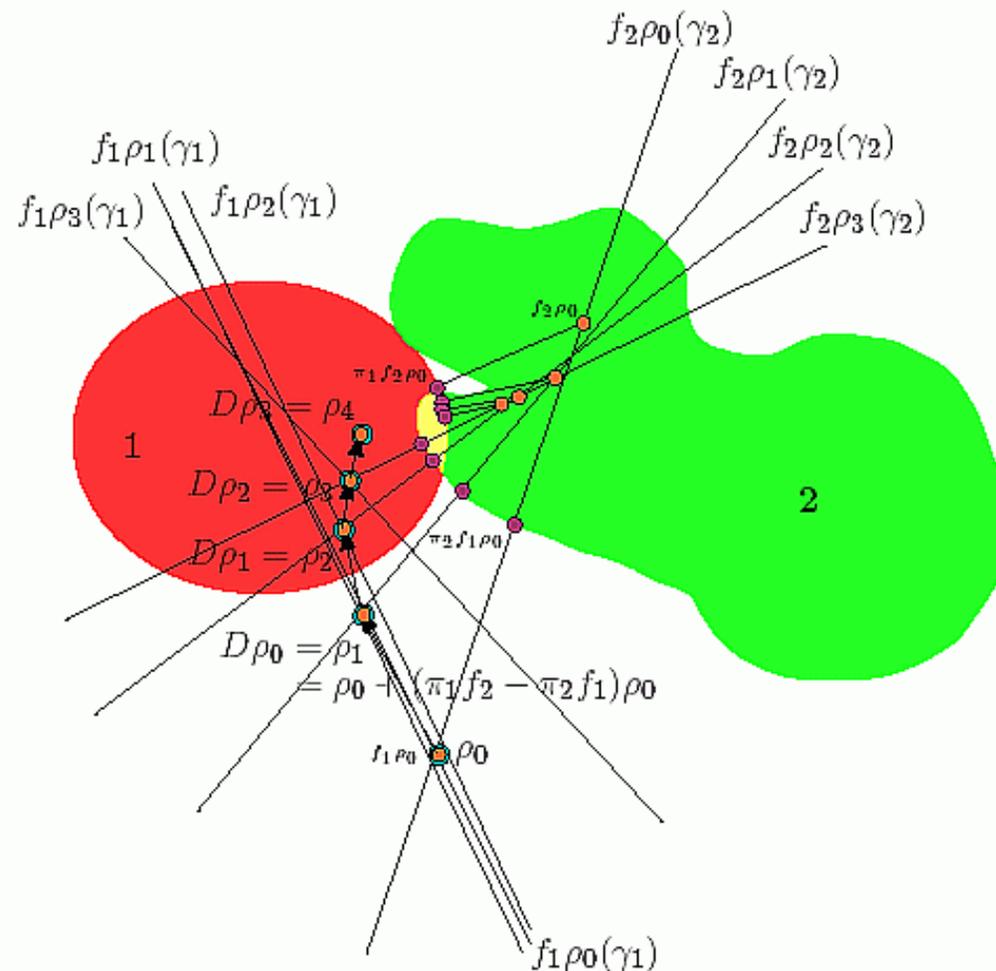
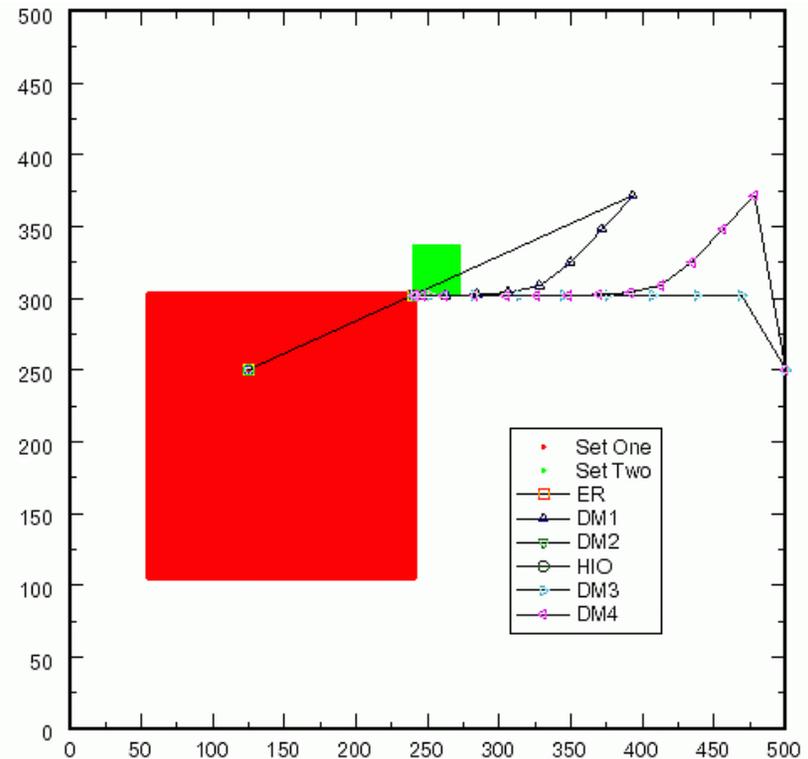
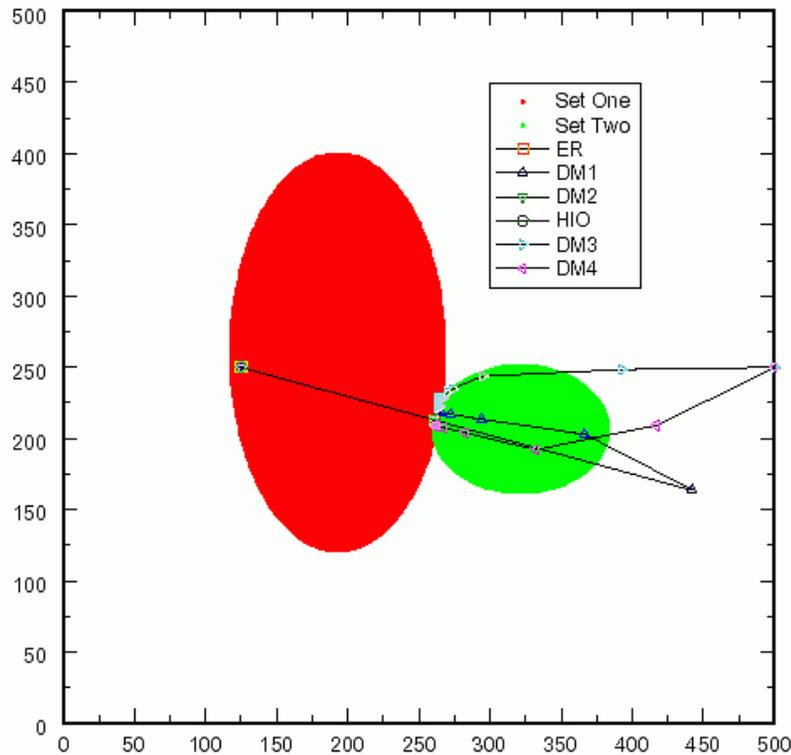


Figure 2.8: The trajectory of DM with  $\beta = 1$ ,  $\gamma_1 = -1$ , and  $\gamma_2 = 1$ . With this choice of parameters, the DM is maximally contractive and corresponds to Fienup's HIO with  $\beta = 1$ .  $f_{i\rho_0}(\gamma_i)$  is the line connecting  $\rho_0$  with  $\pi_i \rho_0$

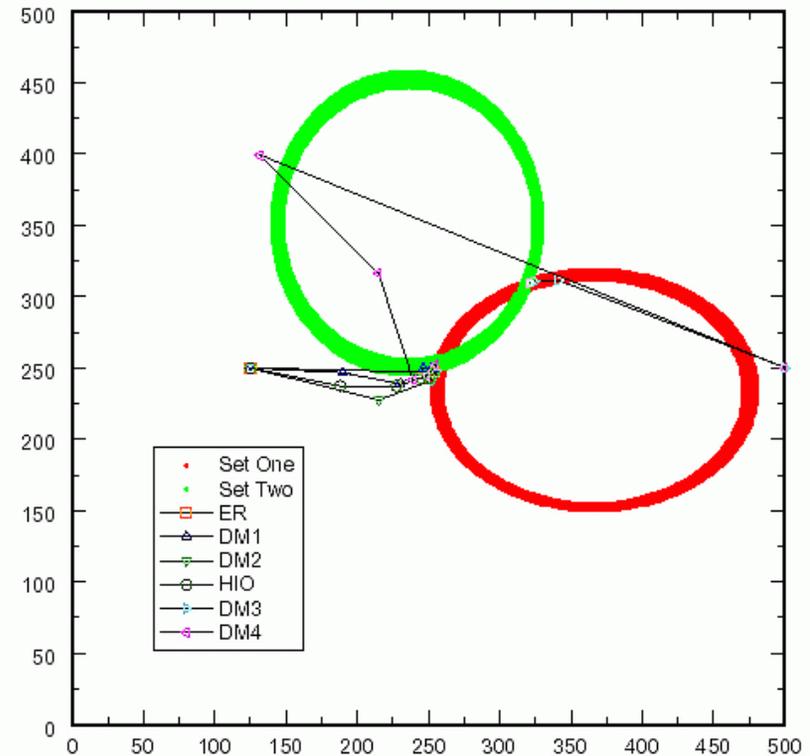
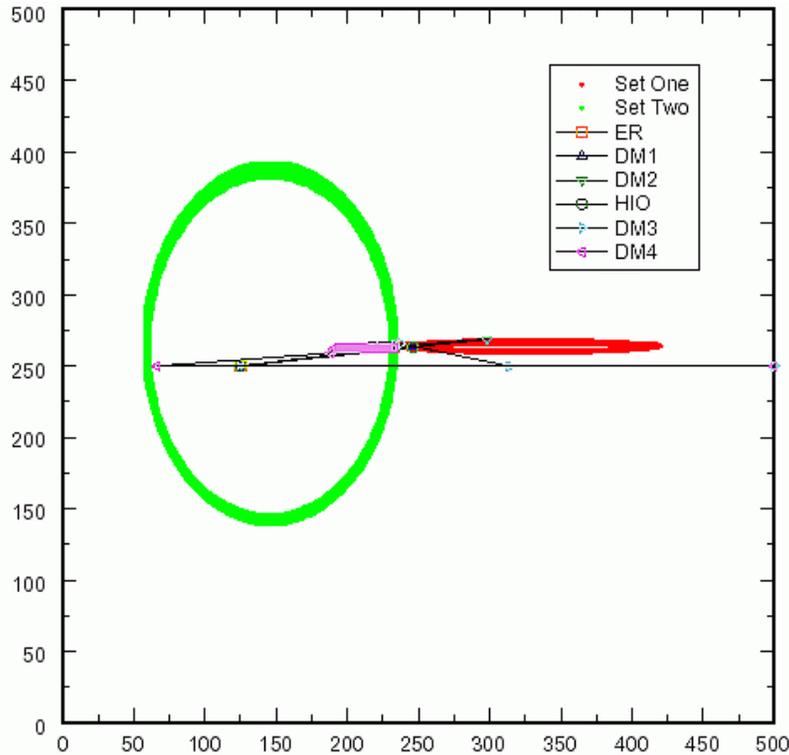
# Trajectoires d'Algorithme



Label	Algorithm	Start x	Start y	Iterations	$\beta$	$\gamma_1$	$\gamma_2$
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	$\beta$	$\gamma_1$	$\gamma_2$
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

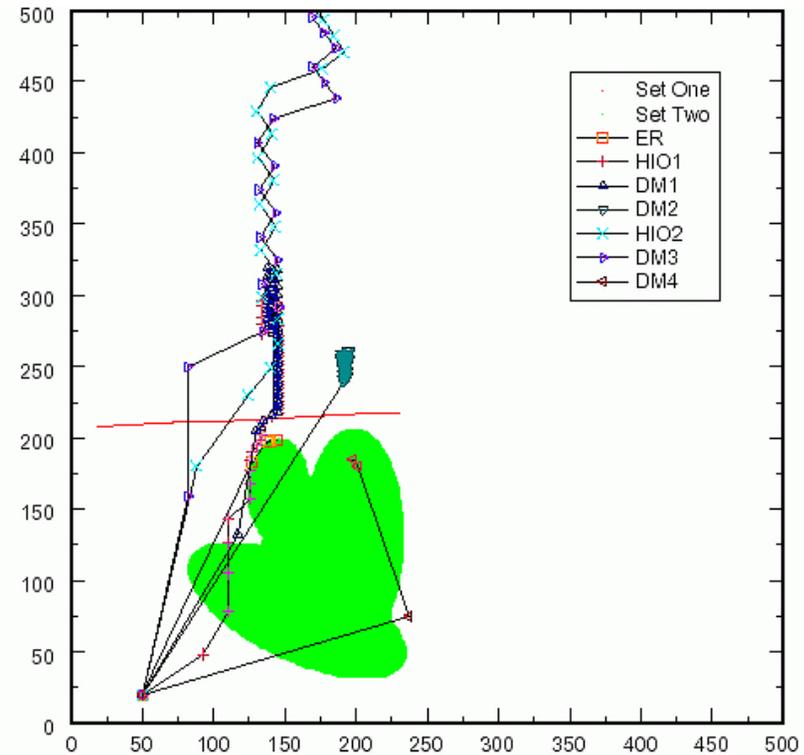
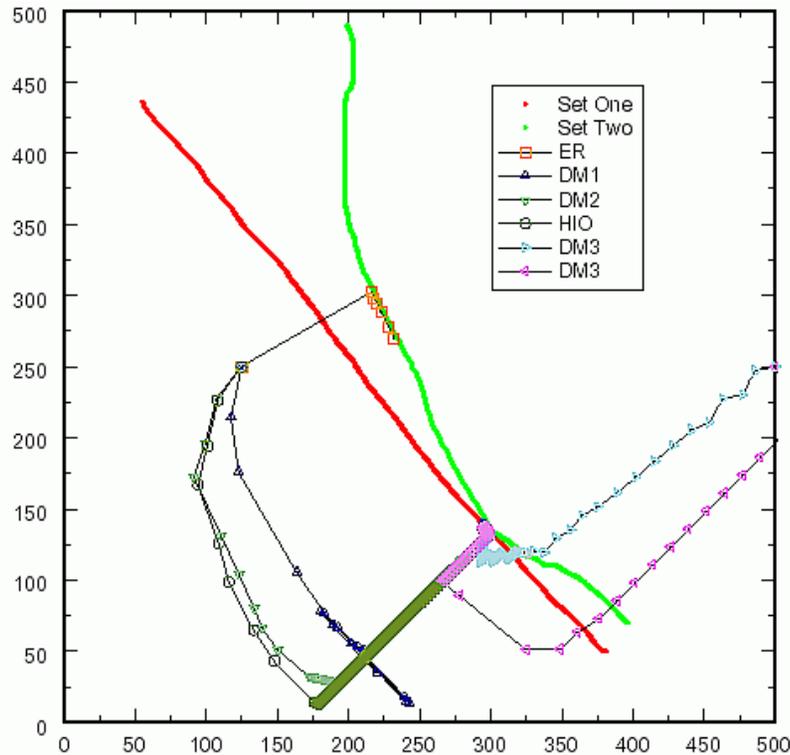
# Trajectoires d'Algorithme



Label	Algorithm	Start x	Start y	Iterations	$\beta$	$\gamma_1$	$\gamma_2$
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	$\beta$	$\gamma_1$	$\gamma_2$
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

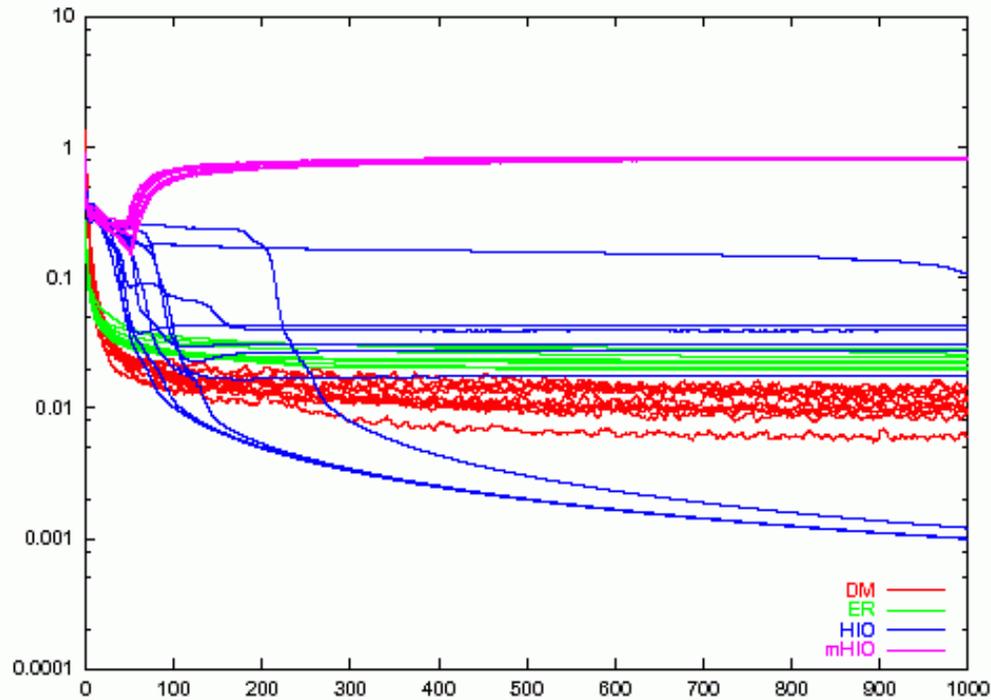


Label	Algorithm	Start x	Start y	Iterations	$\beta$	$\gamma_1$	$\gamma_2$
ER	ER	125	250	50	-	-	-
DM1	DM	125	250	50	0.7	-1	3.33
DM2	DM	125	250	50	0.7	-1.43	1.43
HIO	DM	125	250	50	0.7	-1	1.43
DM3	DM	500	250	50	0.1	-10	10
DM4	DM	500	250	50	0.7	-1	3.33

Label	Algorithm	Start x	Start y	Iterations	$\beta$	$\gamma_1$	$\gamma_2$
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

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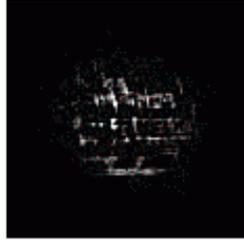


# Convergence: écriture

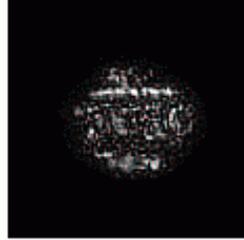
Original



ER



DM



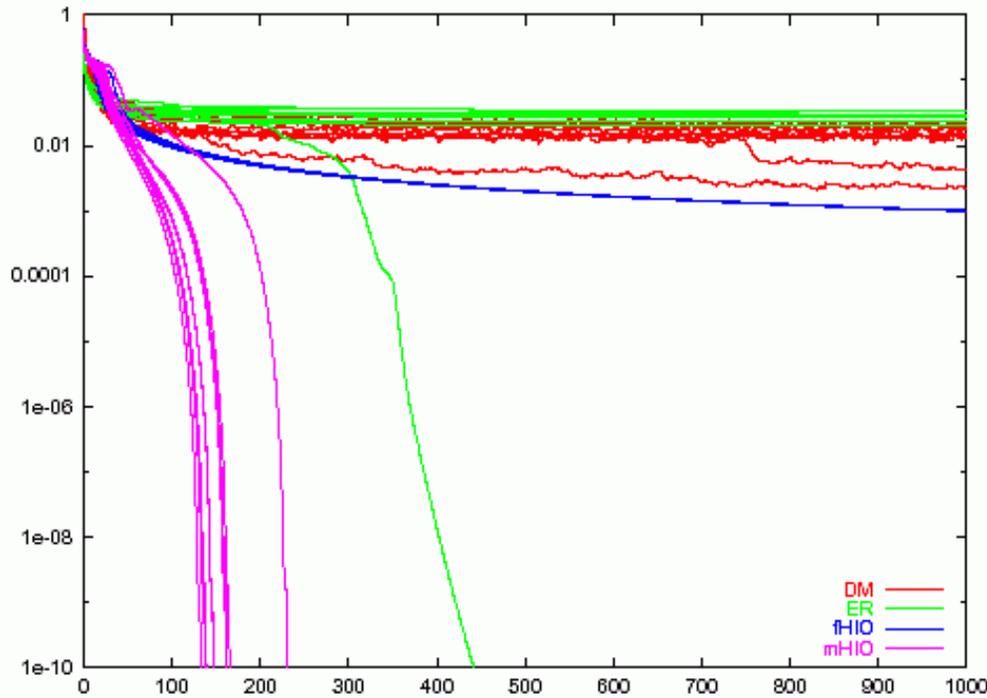
HIO



mHIO

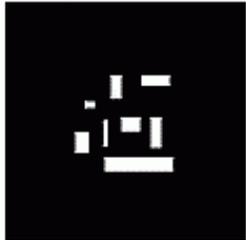


- $\xi_1^2 = 1.2718$
- $\xi_1^2 = 0.3684$
- $\xi_1^2 = 4 \times 10^{-9}$
- $\xi_1^2 = 0.4841$

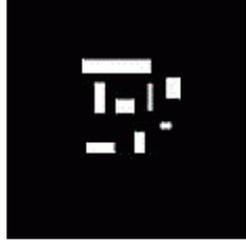


# Convergence: rectangles

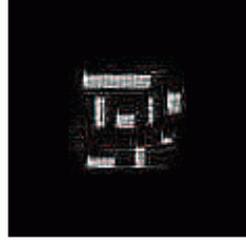
Original



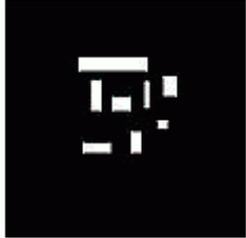
ER



DM



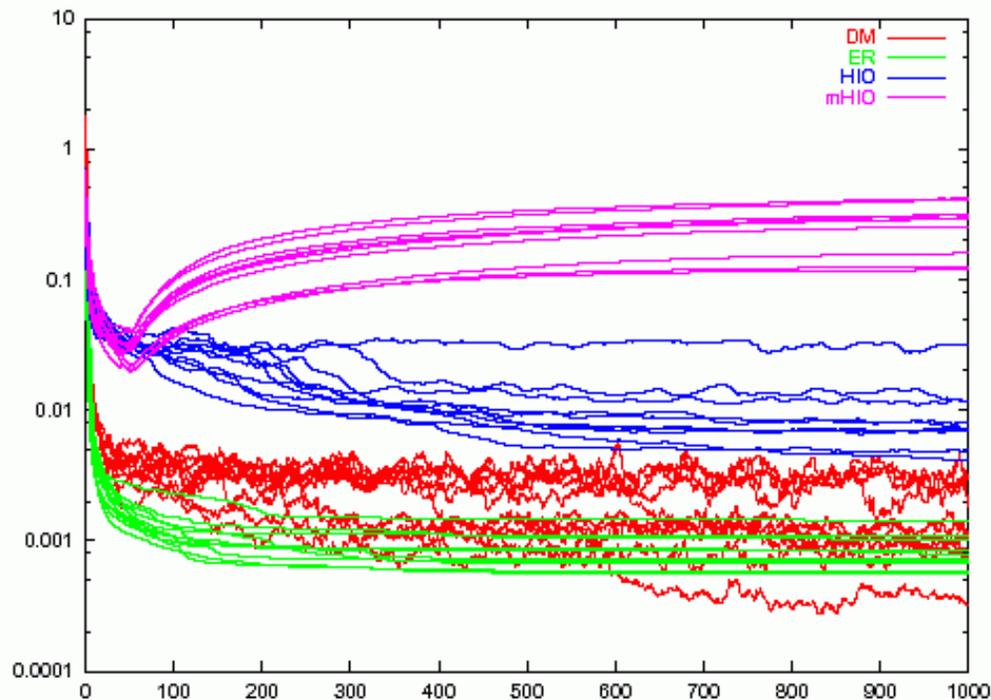
HIO



mHIO

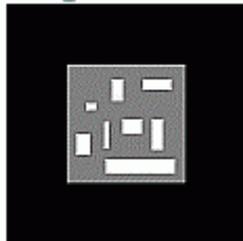


- $\xi_1^2 = 1.0749$
- $\xi_1^2 = 0.1711$
- $\xi_1^2 = 6 \times 10^{-9}$
- $\xi_1^2 = 5 \times 10^{-8}$

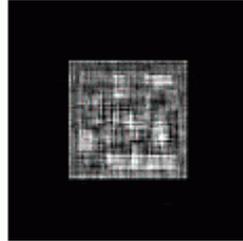


Convergence:  
rectangles  
(échelle grise)

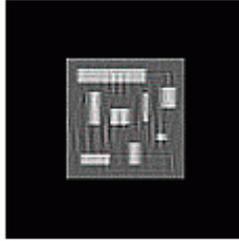
Original



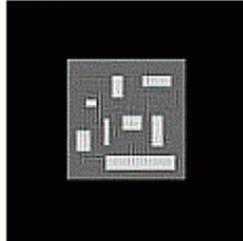
ER



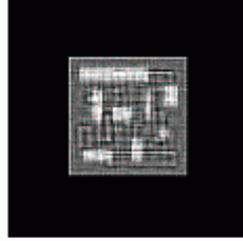
DM



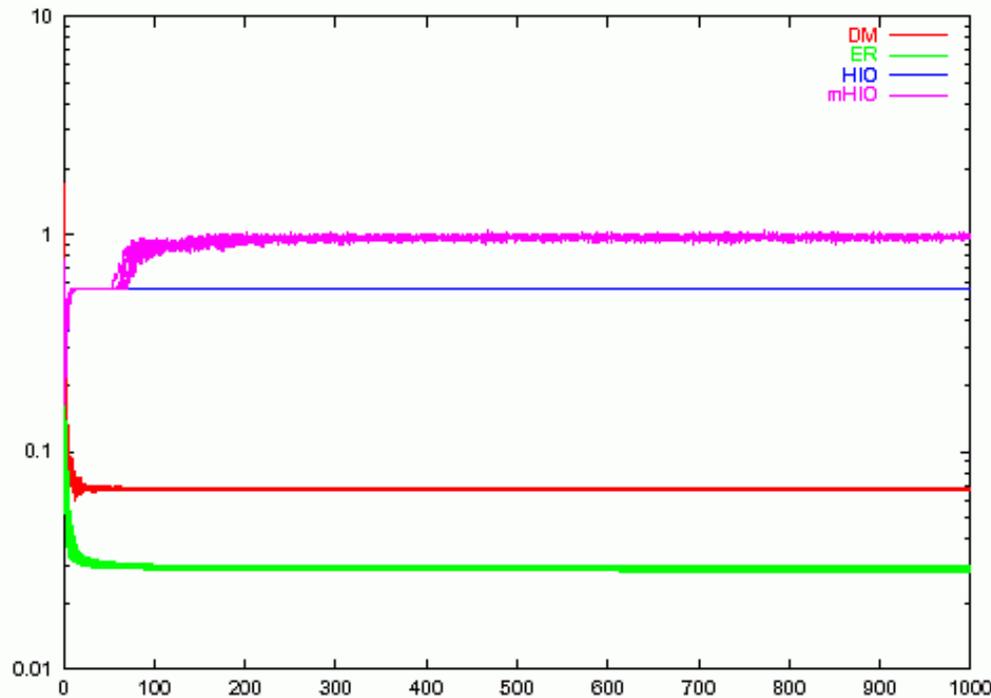
HIO



mHIO

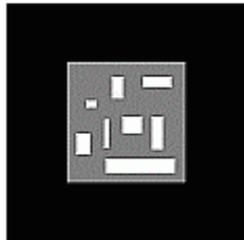


- $\xi_1^2 = 0.0996$
- $\xi_1^2 = 0.0061$
- $\xi_1^2 = 0.0051$
- $\xi_1^2 = 0.0161$

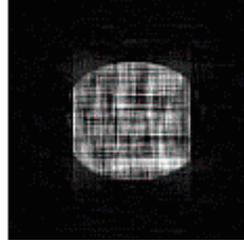


Convergence:  
 rectangles  
 (échelle grise)  
 Support est  
 trop petit

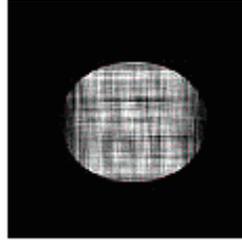
Original



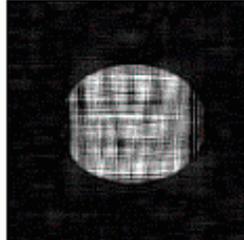
ER



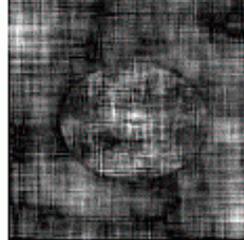
DM



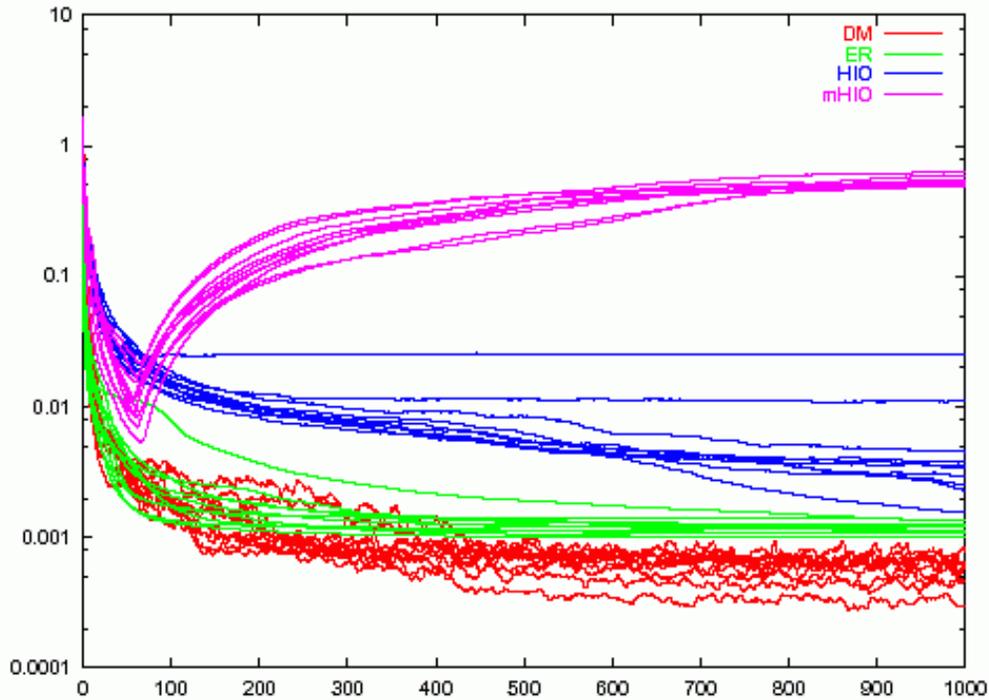
fHIO



mHIO

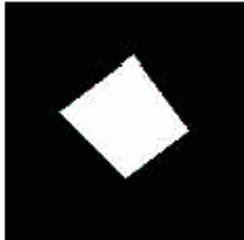


- $\xi_1^2 = 0.1942$
- $\xi_1^2 = 0.0594$
- $\xi_1^2 = 0.1805$
- $\xi_1^2 = 0.3924$

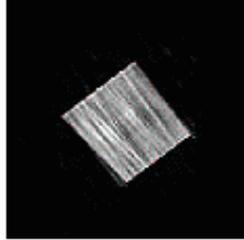


Convergence:  
polygone

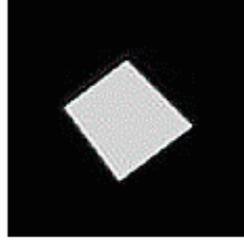
Original



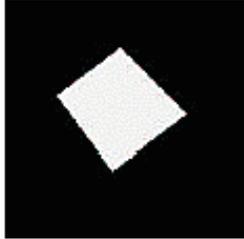
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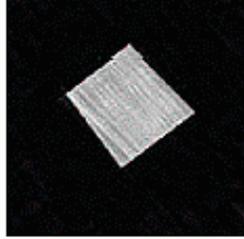
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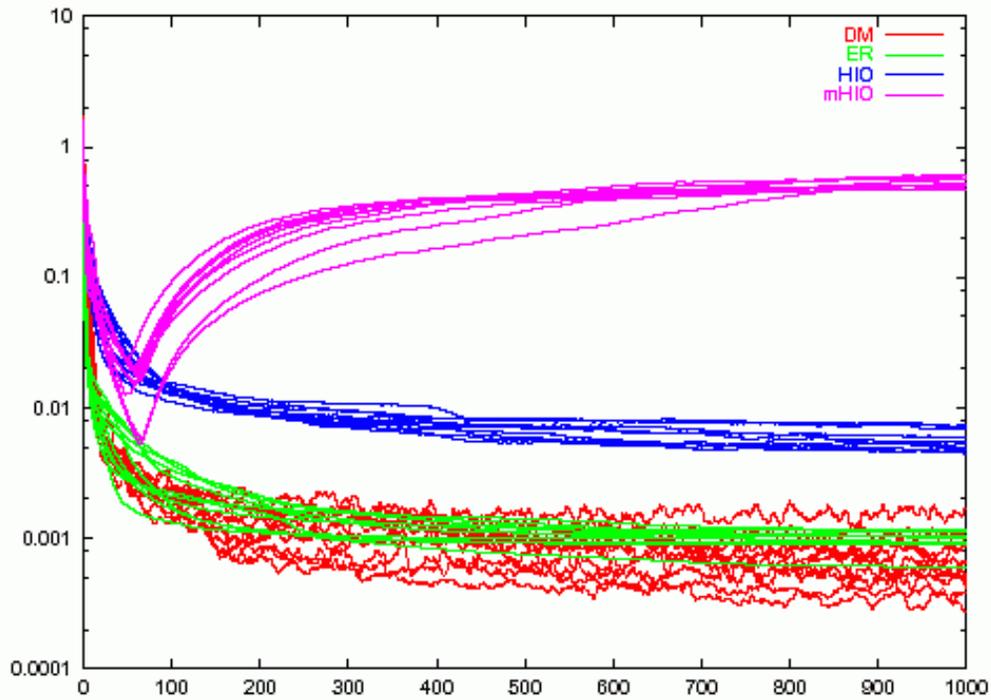
HIO



mHIO

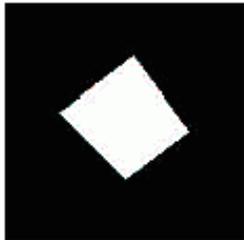


- $\xi_1^2 = 0.0978$
- $\xi_1^2 = 0.0147$
- $\xi_1^2 = 0.0002$
- $\xi_1^2 = 0.0800$

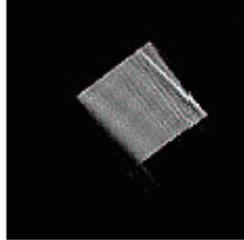


Convergence:  
polygone  
Support Oval

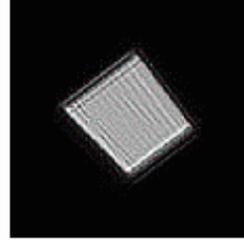
Original



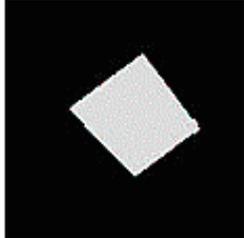
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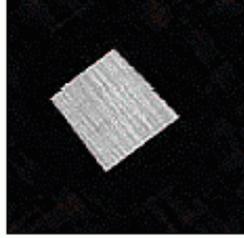
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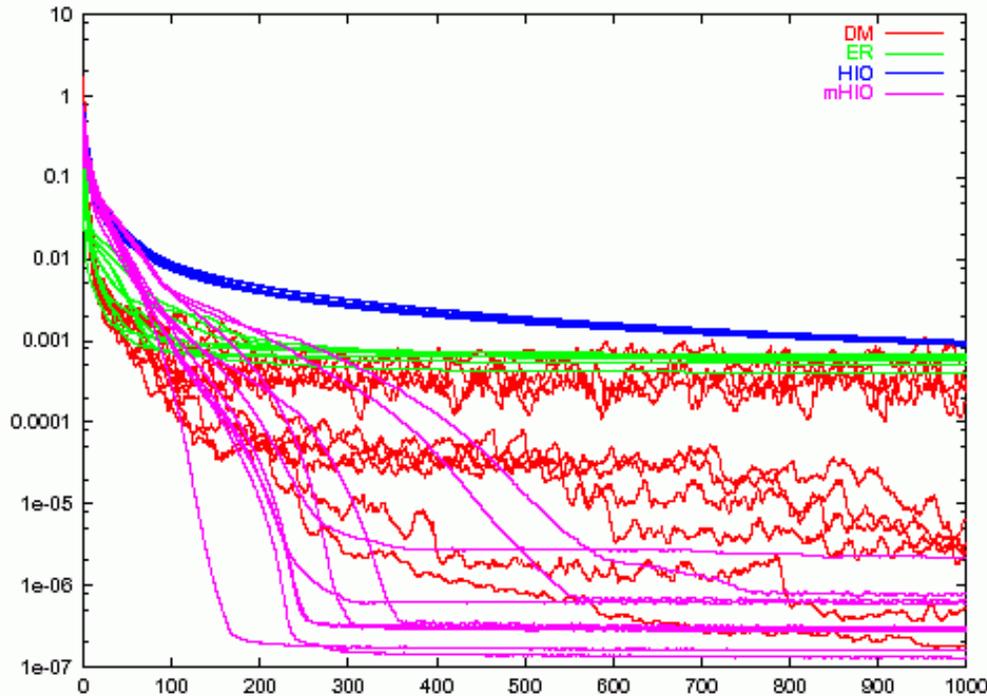
HIO



mHIO

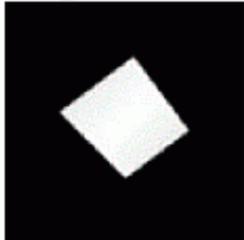


- $\xi_1^2 = 0.0789$
- $\xi_1^2 = 0.0274$
- $\xi_1^2 = 0.0031$
- $\xi_1^2 = 0.1220$

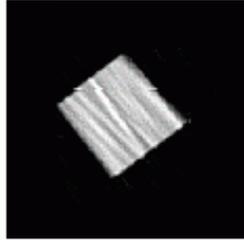


Convergence:  
polygone  
Bords rugueux

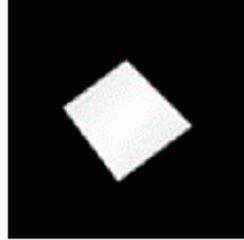
Original



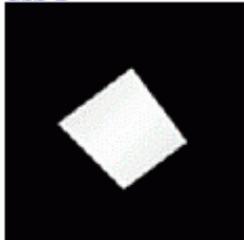
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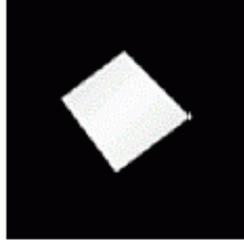
DM



HIO



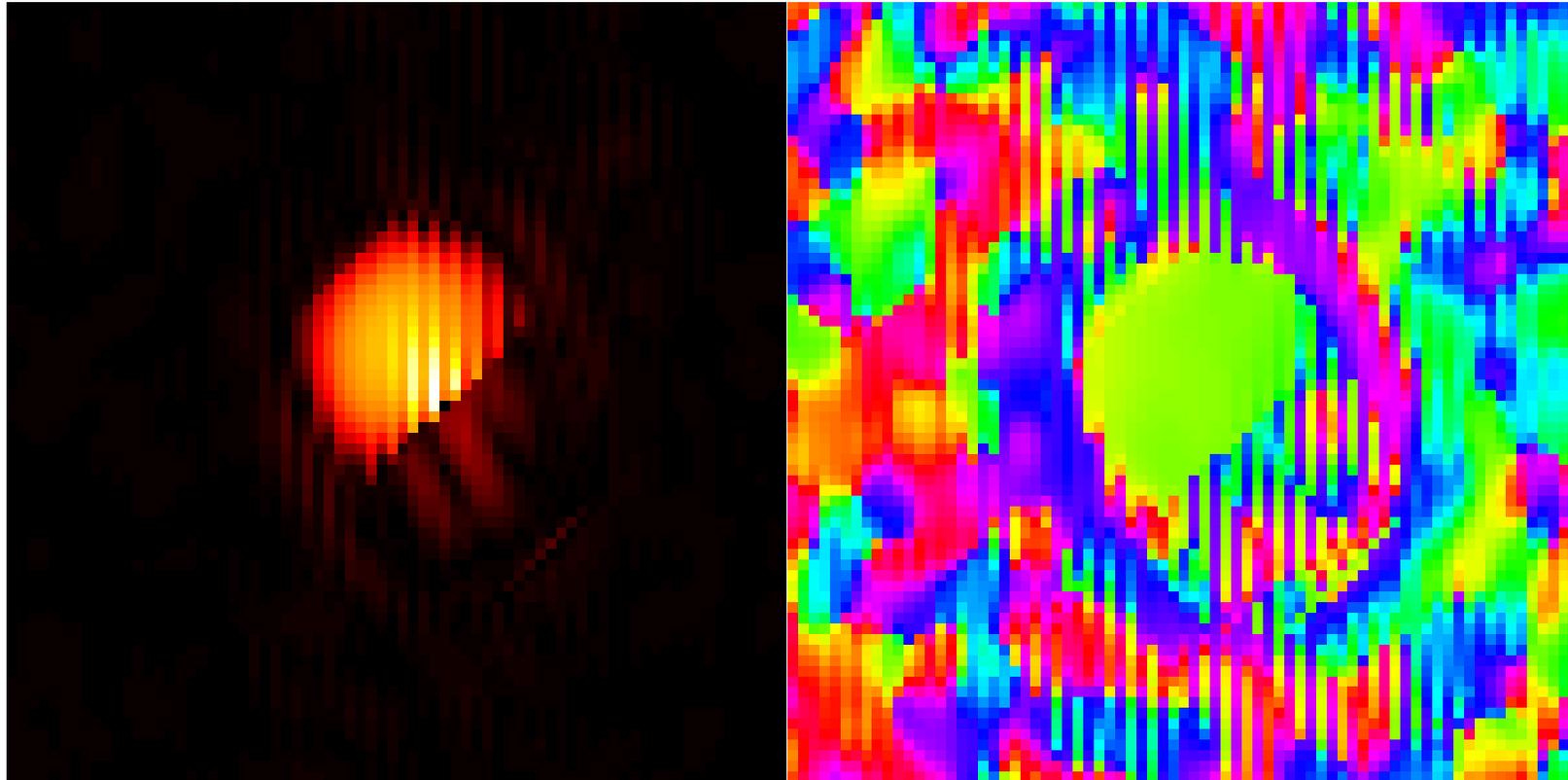
mHIO



- $\xi_1^2 = 0.0158$
- $\xi_1^2 = 5 \times 10^{-5}$
- $\xi_1^2 = 1 \times 10^{-6}$
- $\xi_1^2 = 2 \times 10^{-5}$

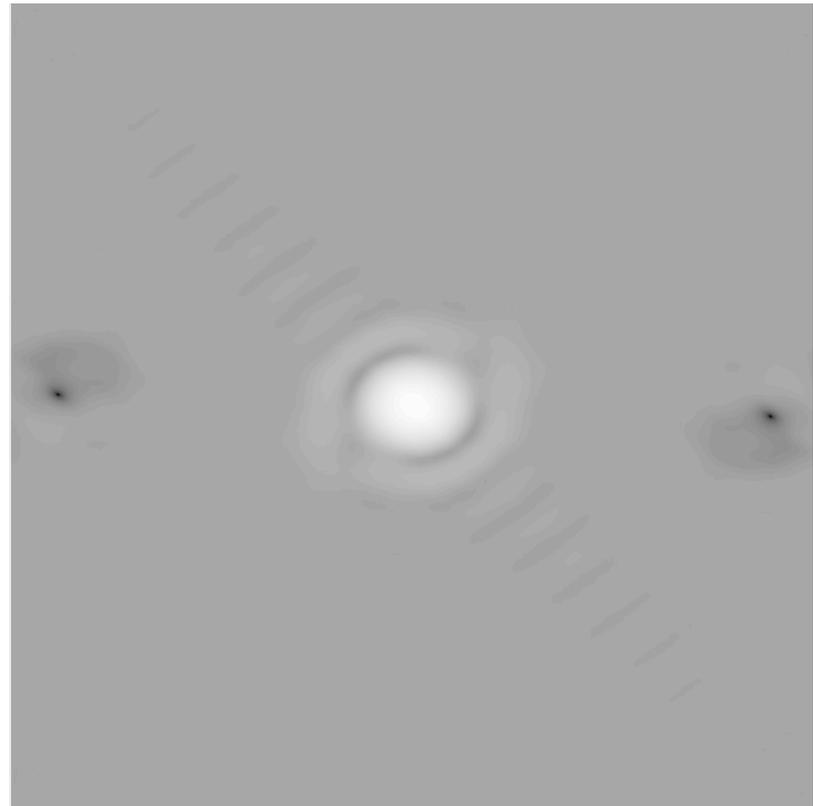
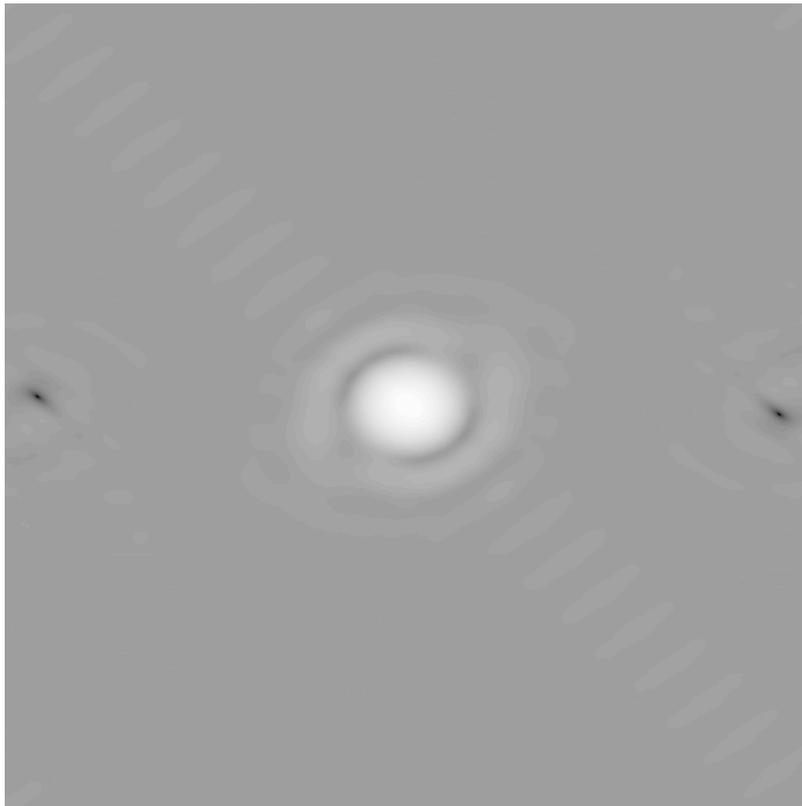
# Reconstruction imparfait peut être rayé

0.5 micron Pb cristal sur SiO<sub>2</sub> substrate



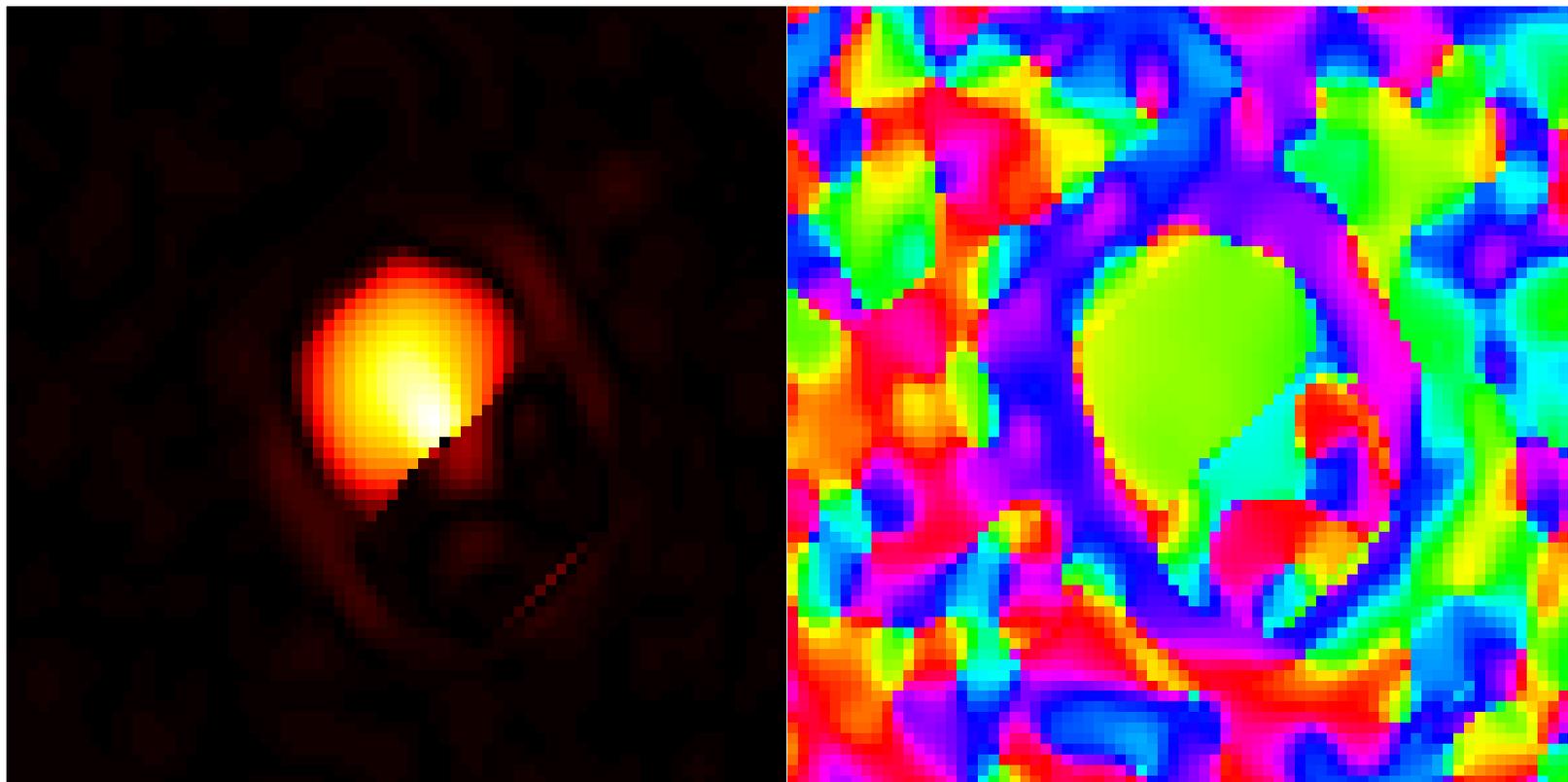
# Image rayé attribué aux “Vortices”

Vortex pairs separated by inverse of stripe spacing

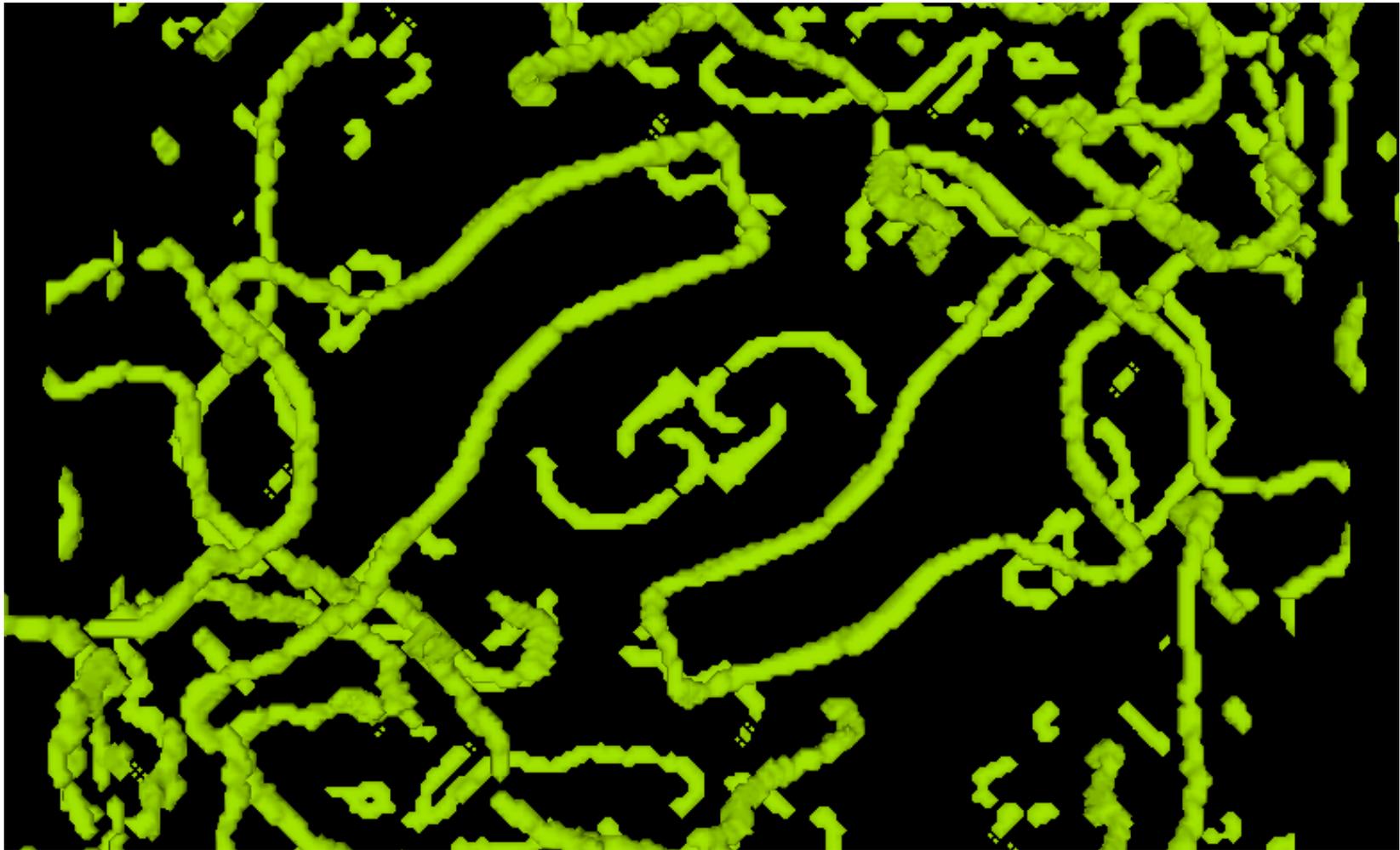


# Result of “Patching” in 2D

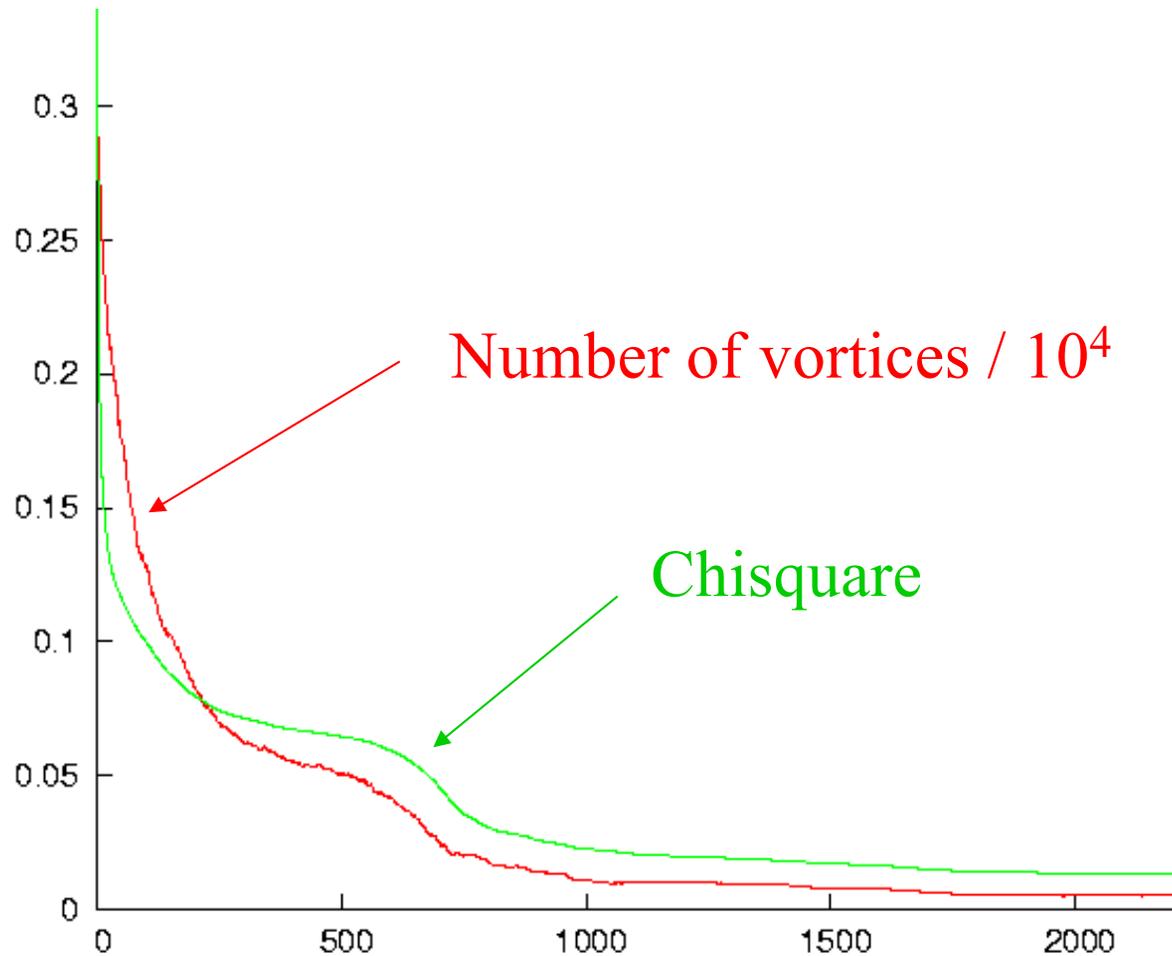
J. R. Fienup Appl. Opt. 21 2758 (1982)



# 3D Vortices Form Pairs of Loops



# Vortices are a Cause of Stagnation during Error Reduction



# Sommaire

- Taille des Nanocristaux
- Unicité
- Algorithmes
- Convergence
- Vortices
- Thèse de Garth Williams:
  - <https://netfiles.uiuc.edu/gjwillms/shared/thesis.pdf>