# Stochastic Optimisation Framework using CIL and SIRF for PET Reconstruction

10th Conference on PET, SPECT, and MR Multimodal Technologies
Total Body and Fast Timing in Medical Imaging

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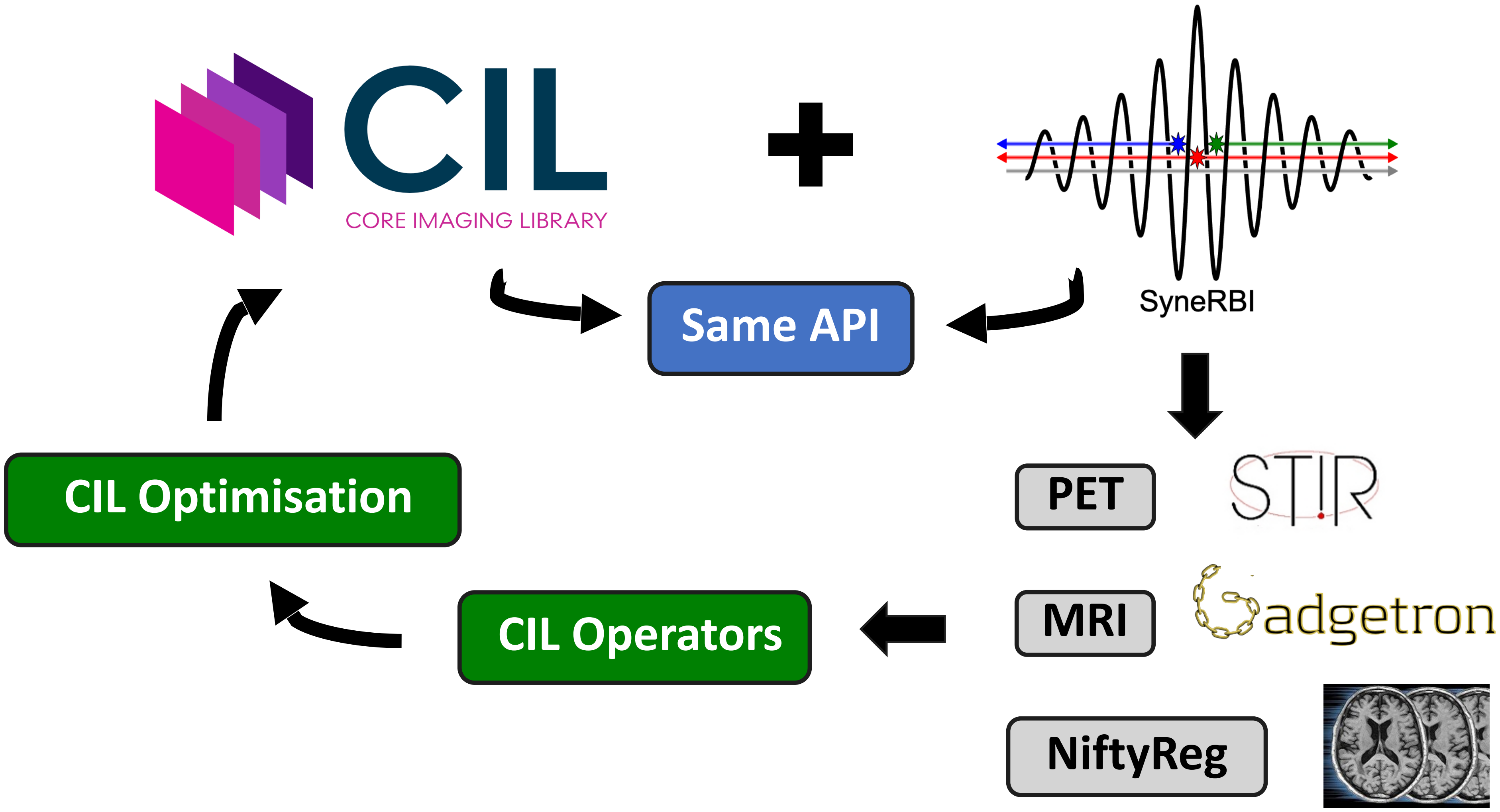
# Overview: CIL and SIRF




*Jørgensen. et al. 2021, Core Imaging Library - Part I: a versatile Python framework for tomographic imaging*
*Papoutsellis et al. 2021, Core Imaging Library - Part II: multichannel reconstruction for dynamic and spectral tomography*
*Ovtchinnikov et al. 2017, SIRF: Synergistic Image Reconstruction Framework*

# Optimisation in CIL

**CIL Optimisation**

⬇

**Functions**

+

**Operators**

=

**Algorithms**

| name | description |
|---|---|
| CGLS | conjugate gradient least squares |
| SIRT | simultaneous iterative reconstruction technique |
| GD | gradient descent |
| FISTA | fast iterative shrinkage-thresholding algorithm |
| LADMM | linearized alternating direction method of multipliers |
| PDHG | primal dual hybrid gradient |
| SPDHG | stochastic primal dual hybrid gradient |

*Chambolle et al 2017, Stochastic Primal-Dual Hybrid Gradient Algorithm with Arbitrary Sampling and Imaging Applications*
*Chambolle et al 2010, A First-Order Primal-Dual Algorithm for Convex Problems with Applications to Imaging*
*Beck et al 2009, A Fast Iterative Shrinkage-Thresholding Algorithm for Linear Inverse Problems*

# Optimisation in CIL

$$\min_x f(x)\ , \quad f: \text{L-smooth}$$

$$\min_x f(x) + g(x)\ , \quad f: \text{L-smooth}\ ,\ g: \text{proximable}$$

$$\min_x f(Kx) + g(x)\ , \quad f: \text{proximable}\ ,\ g: \text{proximable}\ ,\ K \text{ linear operator}$$

$f, g \quad \text{convex}$

***PET reconstruction with Relative Difference Prior***

$$\min_u \sum Au - b\log(Au + \eta) + \mathrm{RDP}(u) + \mathbb{I}_{\{u>0\}}(u)$$

***CT reconstruction with TV regularisation***

$$\min_u \frac{1}{2}\|Au - b\|^2 + \alpha\|\nabla u\|_{2,1} + \mathbb{I}_{\{u>0\}}(u)$$

***TGV denoising Salt and Pepper Noise***

$$\min_u \frac{1}{2}\|u - b\|_1 + \alpha\|\nabla u - w\|_{2,1} + \beta\|\mathcal{E}w\|_{2,1}$$

# Stochastic Project

***Extend CIL Optimisation (Deterministic) framework to Stochastic Optimisation***

**Organised**: CCP SyneRBI , CCPi , PET++

- **1st Hackathon:** November 23-26, 2021
- **2nd Hackathon**: April 4-7, 2022
- **Finden Ltd - Analysis for Innovators (A4i):** Denoising of chemical imaging and tomography data. In collaboration with National Physical Laboratory (05/2023 - 09/2023)

**Joint work**: Kris Thielemans, Gillman Ashley, Tang Junqi, Zeljko Kereta, Imraj Singh, Gemma Fardell, Evgueni Ovtchinnikov, Matthias Ehrhardt, Laura Murgatroyd, Robert Twyman, Edoardo Pasca, Claire Delplancke, Georg Schramm, Daniel Deidda, Jakob Jørgensen, Sam Porter, Margaret Duff, Antony Vamvakeros, Simon Jacques, Casper da Costa-Luis

# Stochastic Project

***<u>Extend CIL Optimisation (Deterministic) framework to Stochastic Optimisation</u>***

- **<u>Implement splitting for CIL/SIRF DataContainers: CT, PET, SPECT, MRI data</u>**
- **<u>Implement randomized algorithms in CIL, e.g., SGD, SAG, SAGA, SVRG and more</u>**
- **<u>Improve CIL optimisation functionality, e.g., step size, preconditioning</u>**

$$\min_x f(x) + g(x) \quad , \quad \min_x f(Kx) + g(x)$$

$$\min_x \sum_{i=1}^{n} f_i(x) + g(x) \quad , \quad \min_x \sum_{i=1}^{n} f_i(K_i x) + g(x)$$


Defazio et al. 2014, SAGA: A Fast Incremental Gradient Method With Support for Non-Strongly Convex Composite Objectives
Schmidt et al. 2017, Minimizing finite sums with the stochastic average gradient
Johnson et al., 2013, Accelerating Stochastic Gradient Descent using Predictive Variance Reduction

# Stochastic Optimisation in CIL

$$\min_{x} f(x) + g(x)$$

| GD | PGA/ISTA | APGA/FISTA |
| --- | --- | --- |
| $x_{k+1} = x_k - \gamma_k \nabla f(x_k)$ | $x_{k+1} = \mathrm{prox}_{\gamma_k g}(x_k - \gamma_k \nabla f(x_k))$ | $x_{k+1} = \mathrm{prox}_{\gamma_k g}(y_k - \gamma_k \nabla f(y_k))$ <br> $\alpha_{k+1} = \frac{1 + \sqrt{1 + 4\alpha_k^2}}{2}$ <br> $y_k = x_k + \frac{\alpha_k - 1}{a_{k+1}}(x_k - x_{k-1})$ |

# Stochastic Optimisation in CIL

$$\min_x \sum_{i=1}^{n} f_i(x) + g(x)$$

**_- Avoid computing the full gradient per iteration, i.e., gradient for all n._**

**_- Select a random index_** $i_k \in \{1,\ldots,n\}$ **_and compute_** $\nabla f_{i_k}$ **_per iteration._**

| GD | PGA/ISTA | APGA/FISTA |
|---|---|---|
| $x_{k+1} = x_k - \gamma_k \nabla f_{i_k}(x_k)$ | $x_{k+1} = \mathrm{prox}_{\gamma_k g}(x_k - \gamma_k \nabla f_{i_k}(x_k))$ | $x_{k+1} = \mathrm{prox}_{\gamma_k g}(y_k - \gamma_k \nabla f_{i_k}(y_k))$<br>$\alpha_{k+1} = \frac{1+\sqrt{1+4\alpha_k^2}}{2}$<br>$y_k = x_k + \frac{\alpha_k - 1}{a_{k+1}}(x_k - x_{k-1})$ |

# Stochastic Optimisation in CIL

| GD | PGA/ISTA | APGA/FISTA |
|---|---|---|
| $x_{k+1} = x_k - \gamma_k \nabla f_{i_k}(x_k)$ | $x_{k+1} = \text{prox}_{\gamma_k g}(x_k - \gamma_k \nabla f_{i_k}(x_k))$ | $x_{k+1} = \text{prox}_{\gamma_k g}(y_k - \gamma_k \nabla f_{i_k}(y_k))$<br>$\alpha_{k+1} = \frac{1+\sqrt{1+4\alpha_k^2}}{2}$<br>$y_k = x_k + \frac{\alpha_k - 1}{a_{k+1}}(x_k - x_{k-1})$ |
| ***SGD*** | ***Prox-SGD*** | ***Acc-Prox-SGD*** |

**ApproximateGradientSumFunction**

***Stochastic Optimisation Design***

- **CIL Class Function**
- **Selects (randomly)** $i_k \in \{1,\dots,n\}$
- **Computes** $\nabla f_{i_k}$

$$\sum_{i=1}^{n} f_i(x)$$

- **No direct implementation of Stochastic algorithms, e.g., SGD.**
- **Use a deterministic algorithm, e.g., GD, already available in CIL.**
- **Implement a Stochastic Gradient "Functions" or Variance-Reduced "Functions"**
- **Example SGD := GD (CIL Algorithm) + SGFunction (CIL Function)**

# Stochastic Optimisation in CIL

| GD | ISTA | FISTA |
|---|---|---|
| $x_{k+1} = x_k - \gamma_k \tilde{\nabla} f_{i_k}(x_k)$ | $x_{k+1} = \mathrm{prox}_{\gamma_k g}(x_k - \gamma_k \tilde{\nabla} f_{i_k}(x_k))$ | $x_{k+1} = \mathrm{prox}_{\gamma_k g}(y_k - \gamma_k \tilde{\nabla} f_{i_k}(y_k))$ <br> $\alpha_{k+1} = \frac{1+\sqrt{1+\alpha_k^2}}{2}$ <br> $y_{k+1} = x_k + \frac{\alpha_k - 1}{\alpha_{k+1}}(x_k - x_{k-1})$ |

**ApproximateGradientSumFunction**

$$\sum_{i=1}^{n} f_i(x)$$

**Stochastic Gradient and Variance-Reduced CIL "Functions"**

- **SGFunction**
- **SAGFunction**
- **SVRGFunction**
- **SAGAFunction**
- **LSVRGFunction**
- **and more ...**

# Stochastic Optimisation in CIL

## Plug and Play Framework - Different Stochastic Gradient Functions

| Algorithms / Stochastic Function | GD | ISTA | FISTA |
|---|---|---|---|
| SGFunction | SGD | Prox-SGD | Acc-Prox-SGD |
| SAGFunction | SAG | Prox-SAG | Acc-Prox-SAG |
| SAGAFunction | SAGA | Prox-SAGA | Acc-Prox-SAGA |
| SVRGFunction | SVRG | Prox-SVRG | Acc-Prox-SVRG |
| LSVRGFunction | LSVRG | Prox-LSVRG | Acc-Prox-LSVRG |

```
gd = GD(initial=initial, objective_function=f, step_size=step_size,
        update_objective_interval=1, max_iteration=10)
gd.run(verbose=1)

pgd = ISTA(initial=initial, f=f, g=g, step_size=step_size,
        update_objective_interval=1, max_iteration=10)
pgd.run(verbose=1)
```

# Stochastic Optimisation in CIL

## Plug and Play Framework - Different Stochastic Gradient Functions

| Algorithms<br>Stochastic Function | GD | ISTA | FISTA |
|---|---|---|---|
| SGFunction | SGD | Prox-SGD | Acc-Prox-SGD |
| SAGFunction | SAG | Prox-SAG | Acc-Prox-SAG |
| SAGAFunction | SAGA | Prox-SAGA | Acc-Prox-SAGA |
| SVRGFunction | SVRG | Prox-SVRG | Acc-Prox-SVRG |
| LSVRGFunction | LSVRG | Prox-LSVRG | Acc-Prox-LSVRG |

```
sgd = GD(initial=initial, objective_function=SGFunction(fi), step_size=step_size,
         update_objective_interval=1, max_iteration=10)
sgd.run(verbose=1)

prox_sgd = ISTA(initial=initial, f=SGFunction(fi), g=g, step_size=step_size,
         update_objective_interval=1, max_iteration=10)
prox_sgd.run(verbose=1)
```

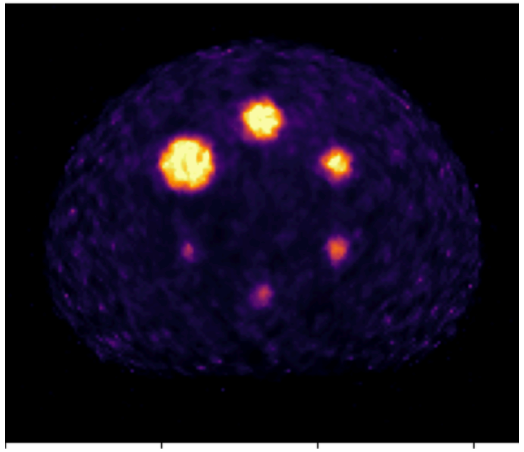
# Stochastic Utilities/Improvements

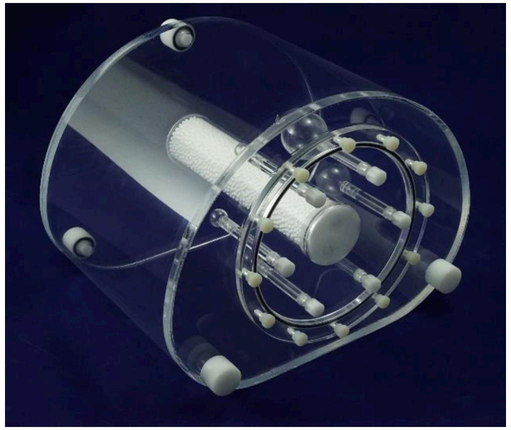
- ✓ **Data splitting methods for AcquisitionData (CIL + SIRF).**
- ✓ **Sampling methods used by Stochastic Functions, i.e., select the next function** $f_{i_k}$
- ✓ **Callable Classes to improve functionality of CIL Algorithms**
- ✓ **Proximal Gradient Algorithm (PGA) : Base class for Proximal Gradient Algorithms, e.g., GD, ISTA, FISTA**
- ✓ **CIL + SIRF fully compatible --> SIRF Functions can be used with CIL Algorithms**

# Stochastic Utilities

## ✓ Example: Data splitting methods for AcquisitionData (CIL + SIRF)

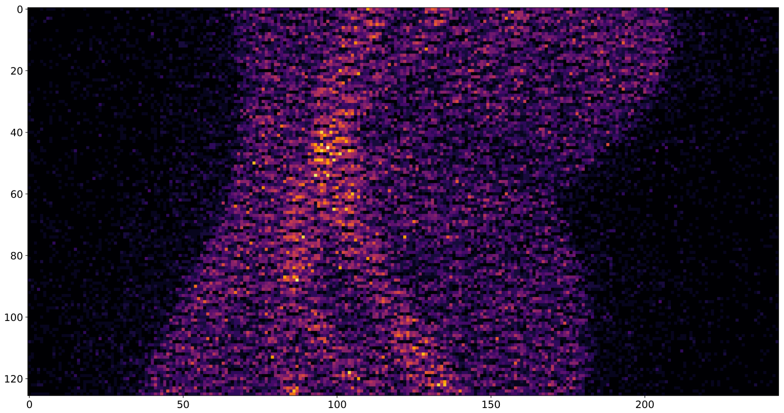
***NEMA dataset***



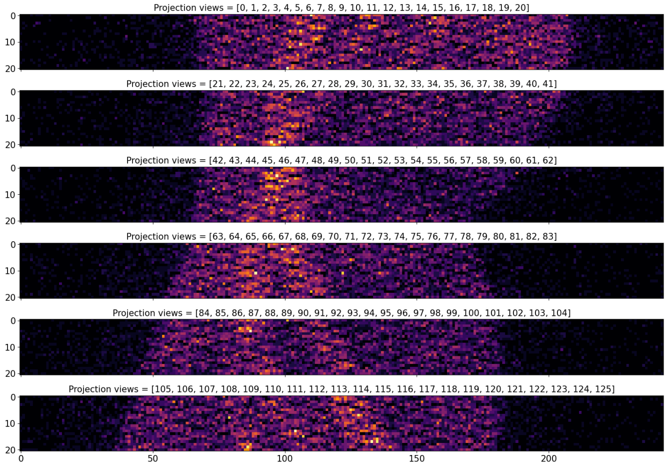


**Split to 6 subsets**

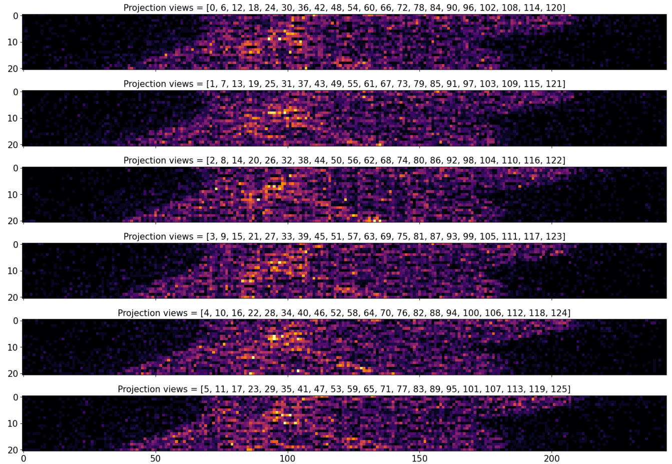
**126 projection views**



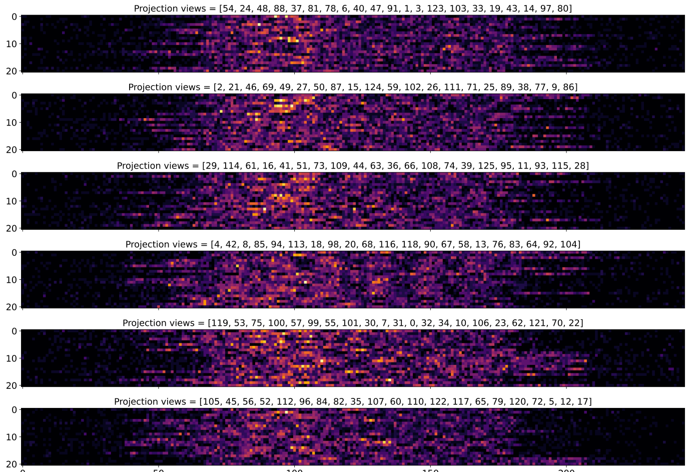

**Ordered (Step_size=1)**




**Ordered (Step_size= NumSubsets )**




**Random**



# Stochastic Utilities

✓ **Example: Sampling methods used from Stochastic Functions**

## Uniform Sampling (With replacement) n=6

| Iteration | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Function | $f_3$ | $f_4$ | $f_0$ | $f_5$ | $f_1$ | $f_4$ | $f_3$ | $f_1$ | $f_4$ | $f_0$ | $f_0$ | $f_1$ |

## RandomShuffle (Without replacement)

| Iteration | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Function | $f_3$ | $f_1$ | $f_0$ | $f_2$ | $f_4$ | $f_5$ | $f_4$ | $f_1$ | $f_0$ | $f_2$ | $f_5$ | $f_3$ |

## SingleShuffle (Without replacement)

| Iteration | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Function | $f_3$ | $f_2$ | $f_4$ | $f_0$ | $f_1$ | $f_5$ | $f_3$ | $f_2$ | $f_4$ | $f_1$ | $f_5$ | $f_3$ |

## HermanMeyer

| Iteration | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Function | $f_0$ | $f_3$ | $f_1$ | $f_4$ | $f_2$ | $f_5$ | $f_0$ | $f_3$ | $f_1$ | $f_4$ | $f_2$ | $f_5$ |

# CIL Improvements

✓ **Example: Proximal Gradient Algorithm (PGA) Base Class**

$$x_{k+1} = \mathrm{prox}_{\gamma g}(x_k - \gamma \nabla f(x_k))$$

$$x_{k+1} = \mathrm{prox}_{\gamma_k g}(x_k - \gamma_k D(x_k) \nabla f(x_k))$$

```
class Preconditioner(ABC)
class StepSizeMethod(ABC)
```

***Nocedal and Wright "Numerical Optimisation"***

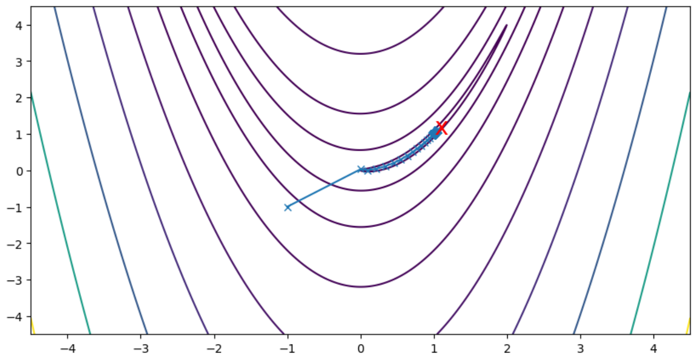
Choose $\bar{\alpha} > 0$, $\rho \in (0, 1)$, $c \in (0, 1)$; Set $\alpha \leftarrow \bar{\alpha}$;
**repeat** until $f(x_k + \alpha p_k) \leq f(x_k) + c\alpha \nabla f_k^T p_k$
$\alpha \leftarrow \rho\alpha$;
**end** (**repeat**)
Terminate with $\alpha_k = \alpha$.

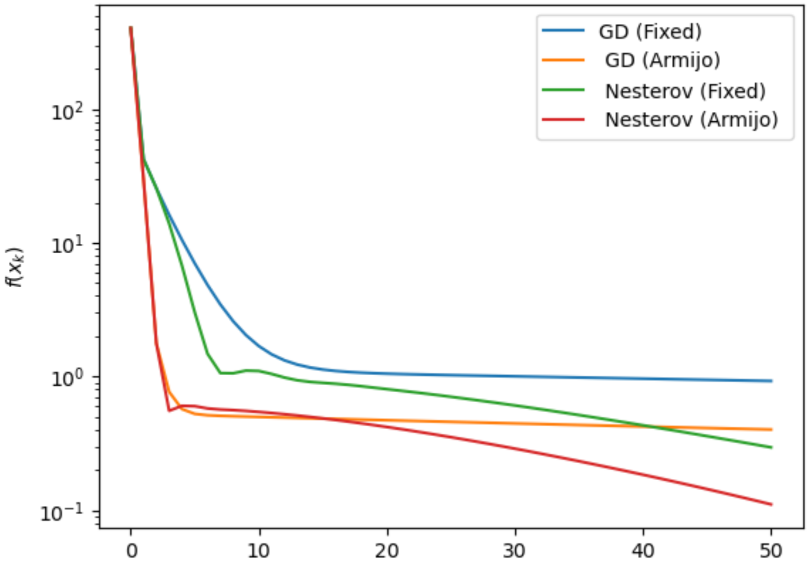
***Armijo condition***

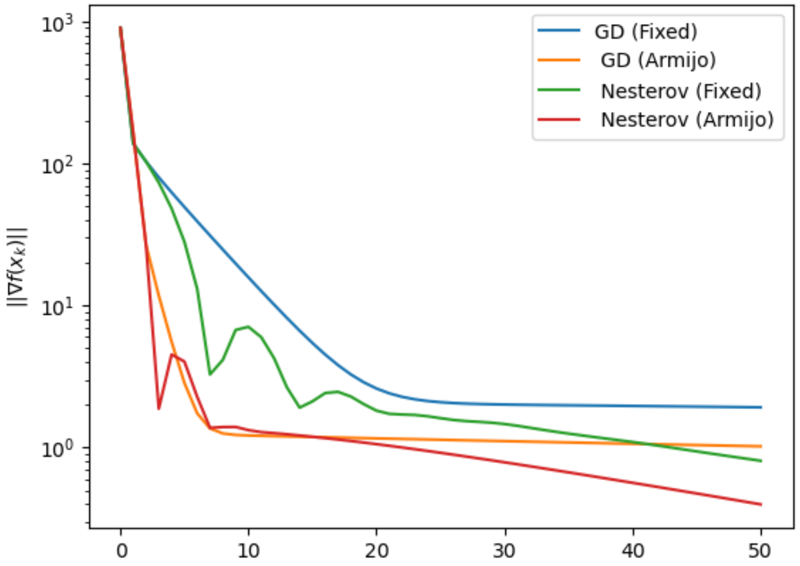
```
armijo = ArmijoStepSize(initial = 1., rho = 0.5, c = 1e-4, iterations=50)
gd = GD(initial = initial, objective_function = f, step_size = armijo,
            max_iteration = 100, update_objective_interval =  1)
gd.run(verbose=1)
```

***Rosenbrock Function: minimum at (x,y) = (1,1)***

$$f(x, y) = (1 - x)^2 + 100(y - x^2)^2$$





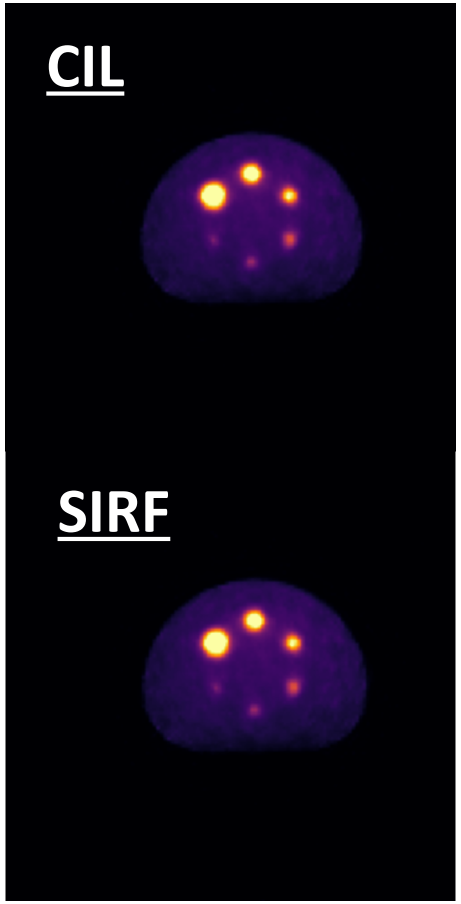
# CIL Improvements

✓ **CIL + SIRF fully compatible** →

```python
class ObjectiveFunction(object)
class Prior(object)
```

$$f(x) = \mathrm{KL}(b, Ax) + \alpha \mathrm{RDP}(x) \quad \rightarrow \quad x_{k+1} = \mathbb{P}_{\geq 0}(x_k - \gamma_k D(x_k) \nabla f(x_k))$$

$$\alpha = 0, \gamma_k = 1$$
$$D(x_k) = \frac{x_k}{A^T \mathbf{1}} \quad \rightarrow \quad x_{k+1} = \frac{x_k}{A^T \mathbf{1}} A^T \left(\frac{d}{Ax_k}\right) \quad (MLEM)$$




**SIRF**

```python
objective = make_Poisson_loglikelihood(d)
objective.set_acquisition_model(A)
objective.set_prior(RelativeDifference)

recon = OSMAPOSLReconstructor()
recon.set_objective_function(objective)
recon.set_num_subsets(1)
recon.set_num_subiterations(50)
recon.set_up(initial)
recon.set_current_estimate(initial)
recon.process()
```

**CIL**

```python
D = AdaptiveSensitivity(A)
pgd = ISTA(initial = initial, f = objective, g = IndicatorBox(lower=0.),
           preconditioner = D, step_size = -1.,
           update_objective_interval=1, max_iteration=50)
pgd.run(verbose=1)
```

# CIL Improvements

✓ **Example: Callable Classes to improve functionality of CIL Algorithms**

```
from cil.optimisation.utilities import MetricsDiagnostics,StatisticsDiagnostics, RSE
from skimage.metrics import structural_similarity as SSIM
from skimage.metrics import normalized_root_mse as NRMSE

cb1 = MetricsDiagnostics(reference_image = fista_1000.solution, verbose=1,
                         metrics_dict={'mae': MAE, 'ssim': SSIM, 'nrmse': NRMSE})
cb2 = StatisticsDiagnostics(verbose=1, statistics_dict={'mean': (lambda x: x.mean())})

fista = FISTA(initial = initial, f = fidelity, g=G, update_objective_interval = 1,
            max_iteration = 5)
fista.run(verbose=1, callback=[cb1, cb2])
```

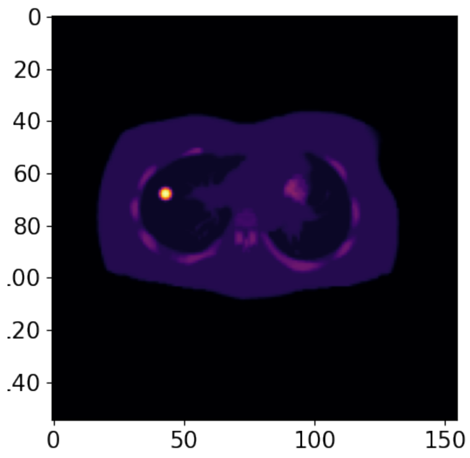
- ***Access to all attributes of the Algorithm***
- ***Define custom metrics (images and/or ROI)***
- ***Define new stopping criteria***
- ***Integrate with Weights and Biases***

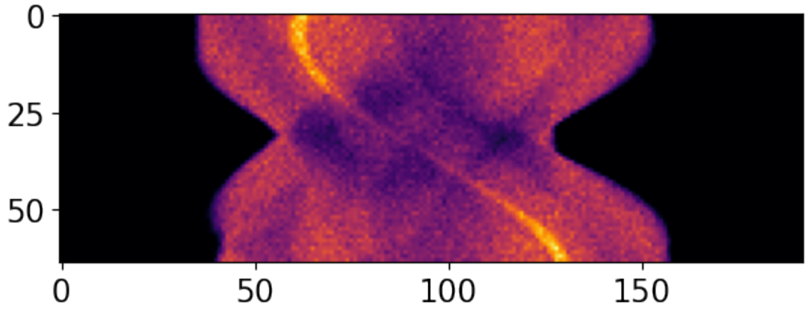
```
     Iter   Max Iter  Time(s)/Iter          Objective              mae             ssim            nrmse             mean
        0          5         0.000       8.17946e+02      6.51097e-05      5.05983e-01      1.00000e+00      0.00000e+00
        1          5         0.542       9.93983e+01      7.07093e-05      2.84027e-01      7.29477e-01      0.00000e+00
        2          5         0.391       7.81449e+01      6.34461e-05      3.14256e-01      6.82127e-01      7.00874e-05
        3          5         0.329       6.22991e+01      5.61340e-05      3.50318e-01      6.37522e-01      6.89979e-05
        4          5         0.297       5.16572e+01      4.95575e-05      3.92073e-01      5.98112e-01      6.79314e-05
        5          5         0.330       4.49825e+01      4.41283e-05      4.37438e-01      5.63993e-01      6.69932e-05
-----------------------------------------------------------------------------------------------------------------------------
Stop criterion has been reached.
```

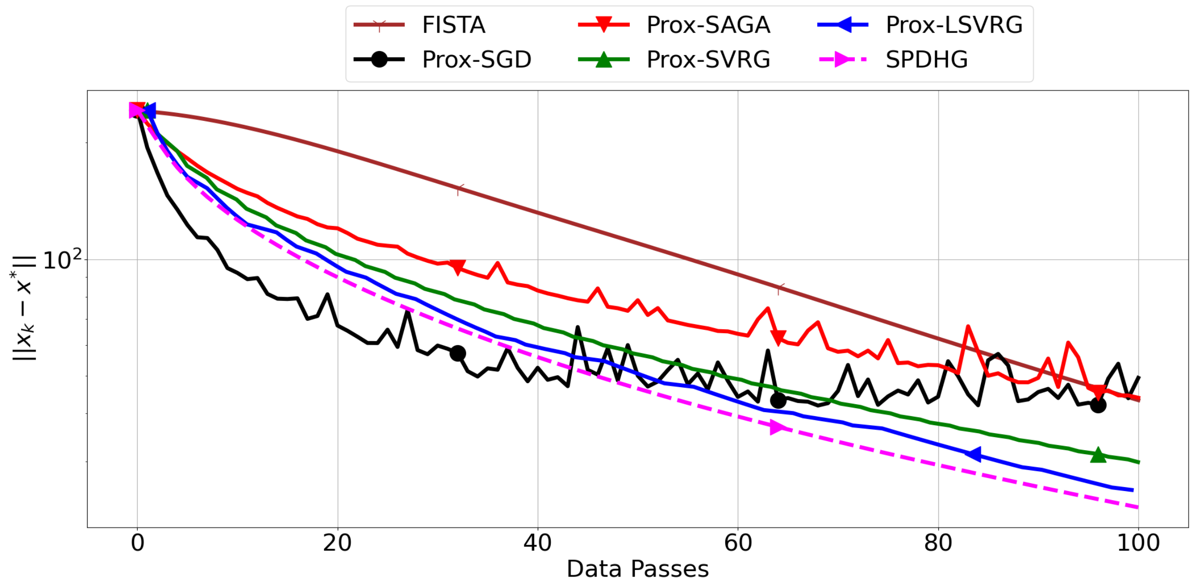
# Applications (PET - Non Smooth optimisation)

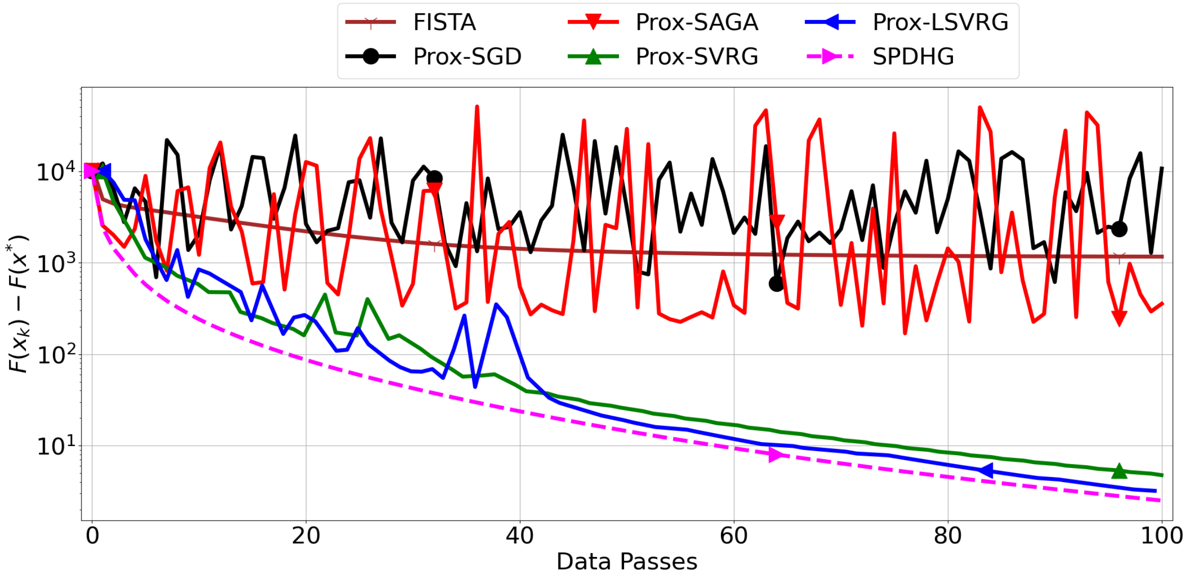
$$\underset{u}{\operatorname{argmin}} \sum Au - b\log(Au + \eta) + \alpha\|\nabla u\|_{2,1} + \mathbb{I}_{\{u>0\}}(u)$$

- **Splitting Method:** Ordered (64 projections), Subsets = 32
- **Sampling Method (Functions):** Random with replacement
- **Optimal Solution:** SPDHG-32 subsets, 500 epochs
- **Step size:** $\gamma_k = \gamma$

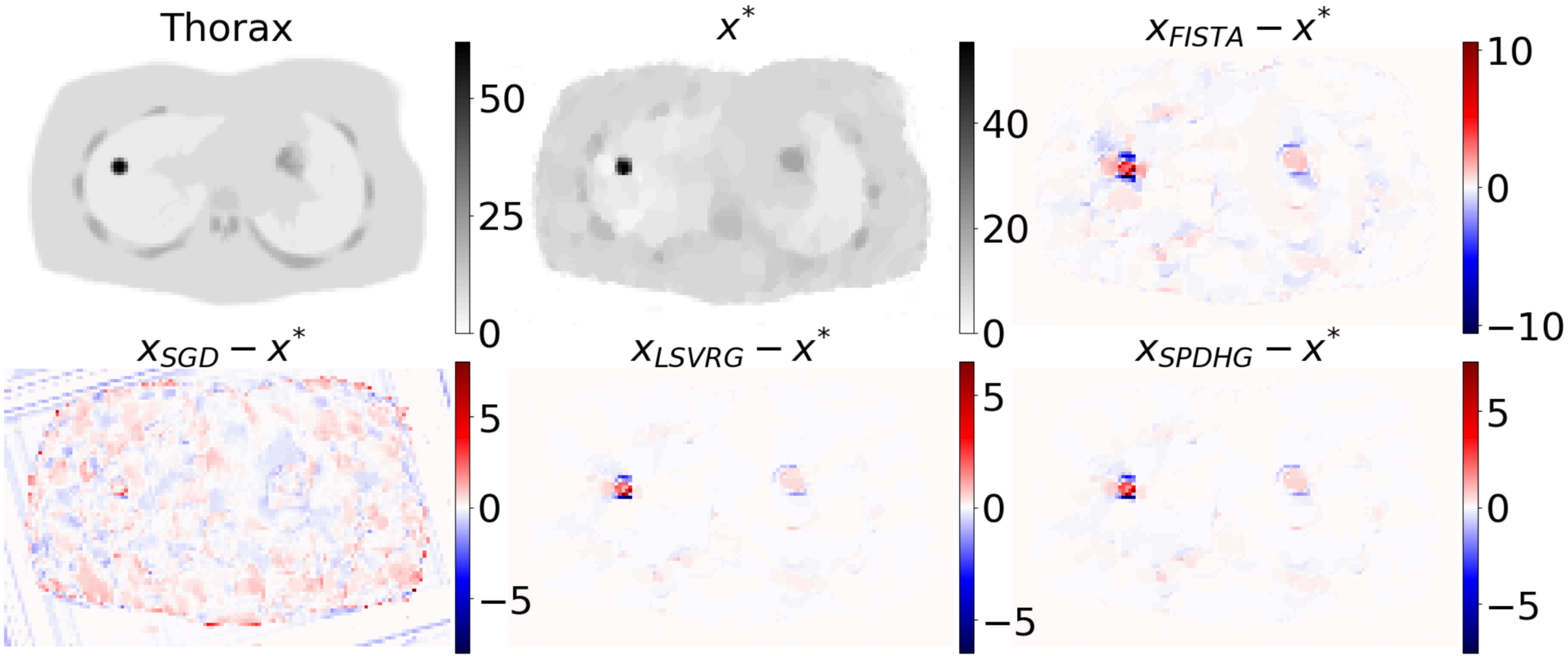






# Applications (PET - Non Smooth optimisation)



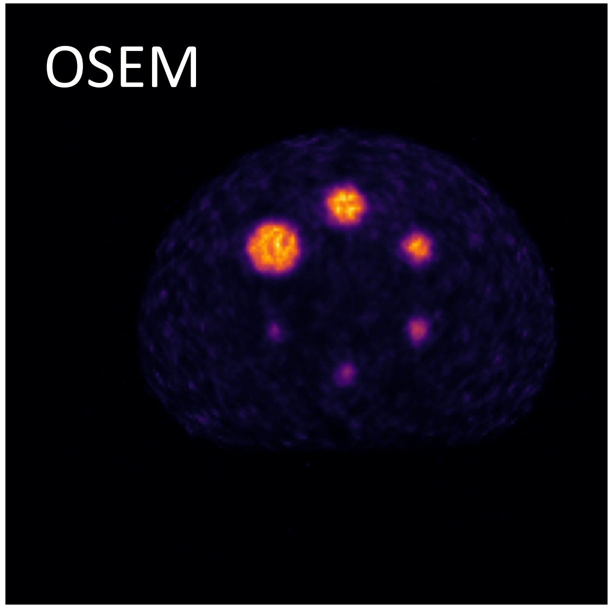
# Applications (PET - Smooth optimisation)

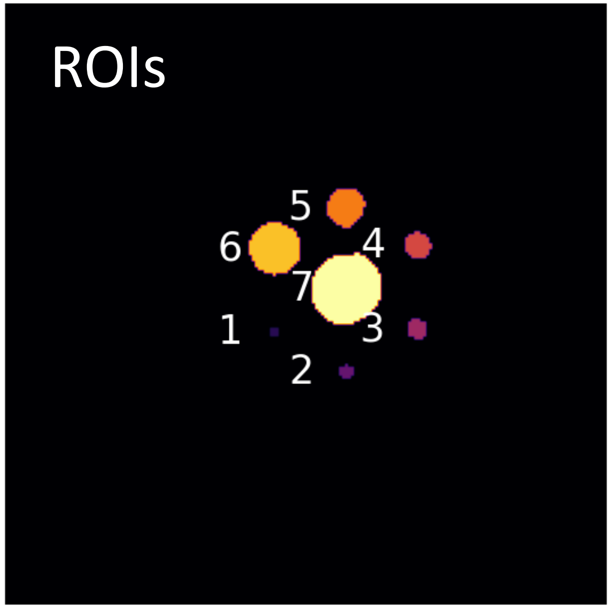
$$\min_u \sum Au - b\log(Au + \eta) + \mathrm{RDP}(u) + \mathbb{I}_{\{u>0\}}(u)$$

- **Splitting Method:** Ordered (126 projections), Subsets = 21, 42, 63
- **Sampling Method (Functions):** Random with replacement
- **Optimal Solution:** (subset) Preconditioned Gradient Descent with relaxed step size, 7 subsets (20000 iterations)
- **Preconditioning:** $D(x_k) = \dfrac{x_{OSEM} + \varepsilon}{A^T 1}$

**Step size:** $\gamma_k = \dfrac{1}{1 + \eta\left(k//(n/2)\right)}$

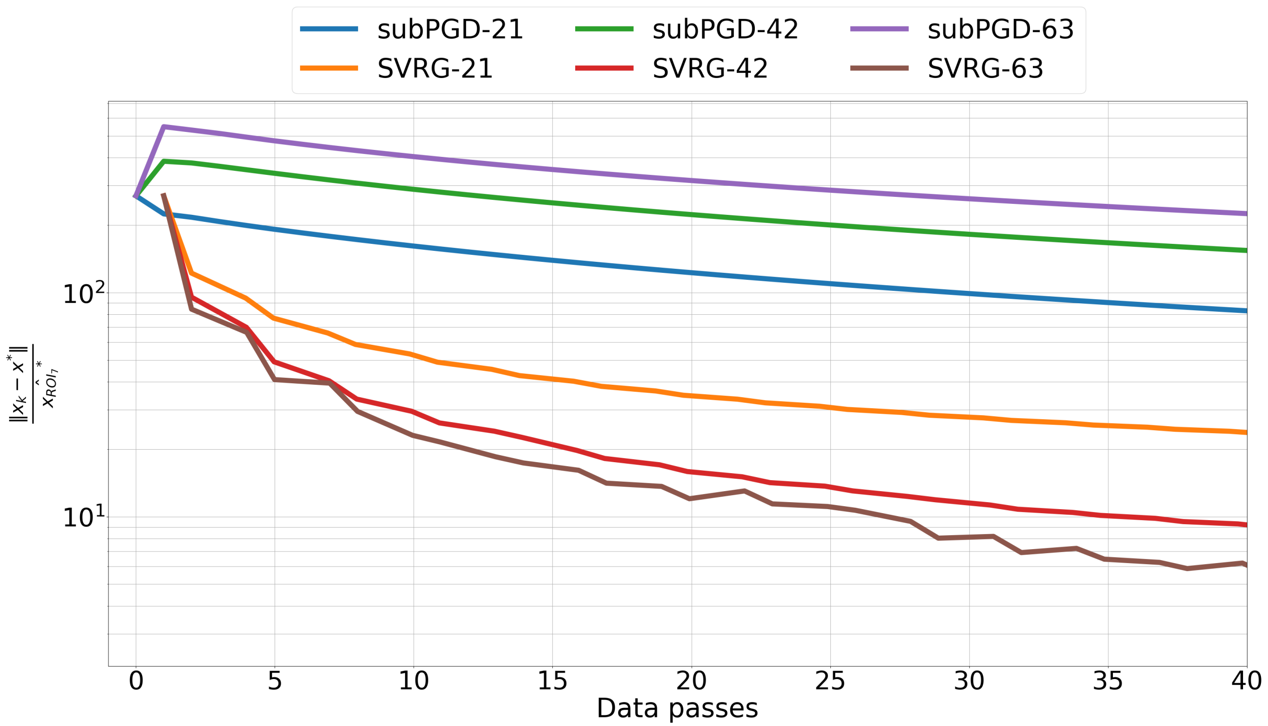
- **Initial:** OSEM

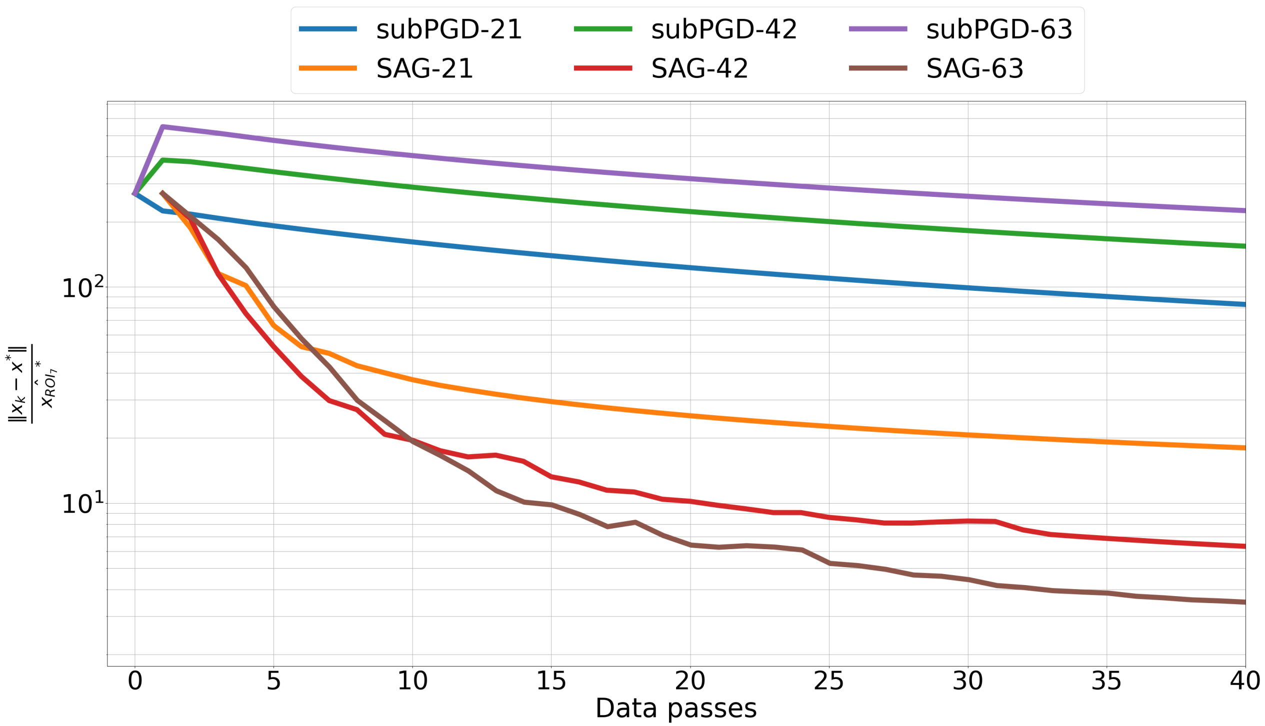


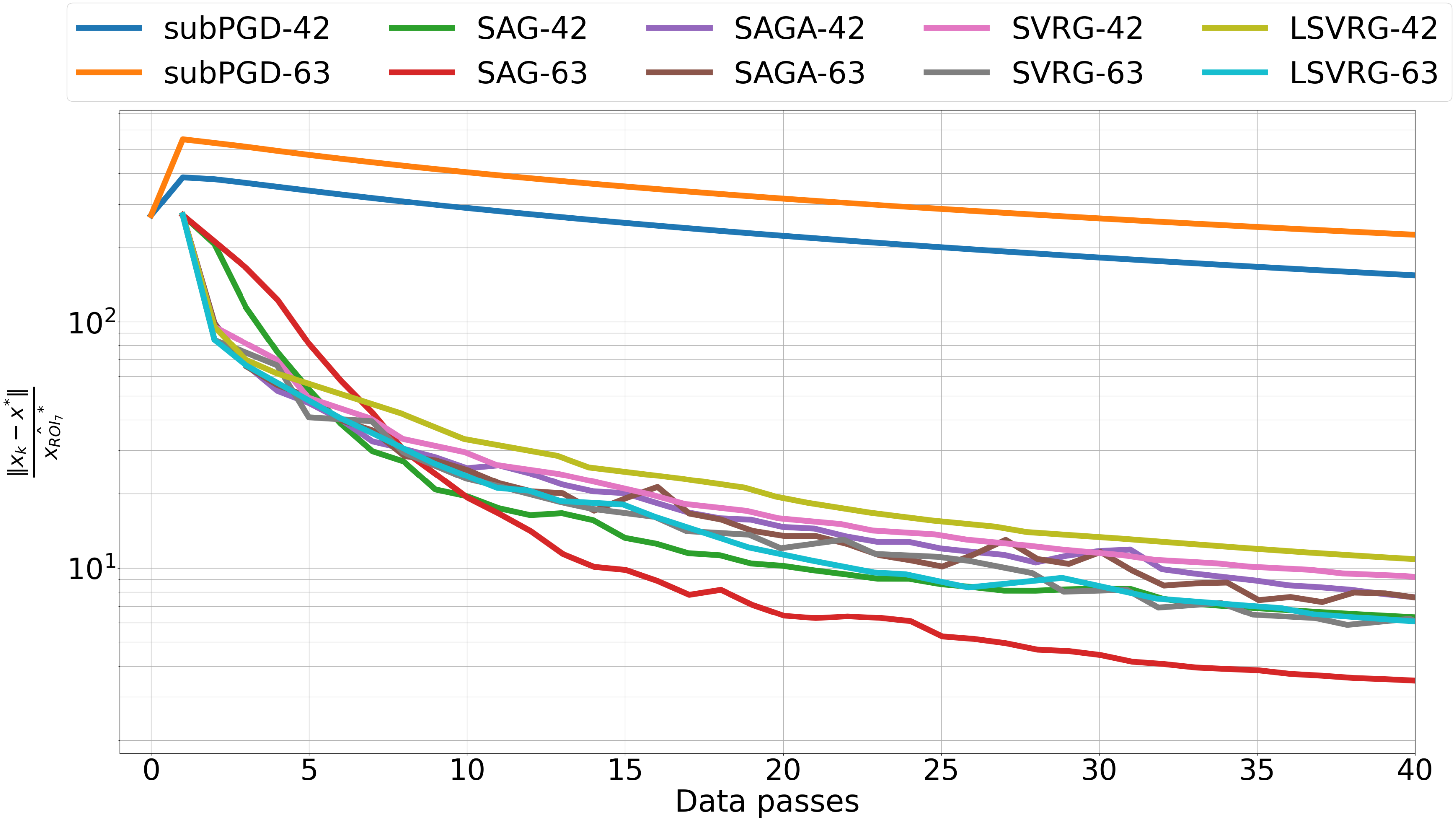

*Twyman et al 2023. An Investigation of Stochastic Variance Reduction Algorithms for 3D Penalised PET Image Reconstruction*

# Applications (PET - Smooth optimisation)

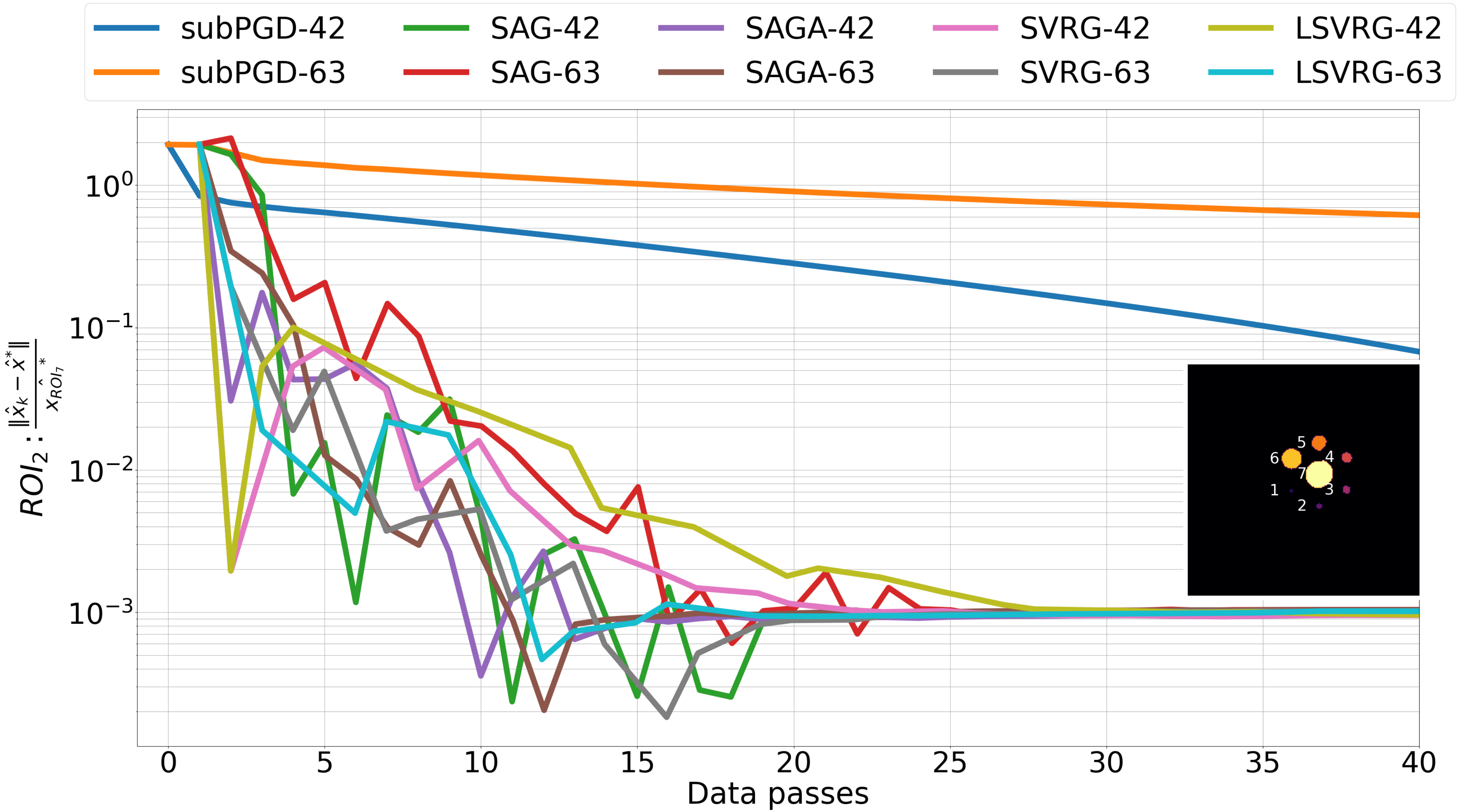


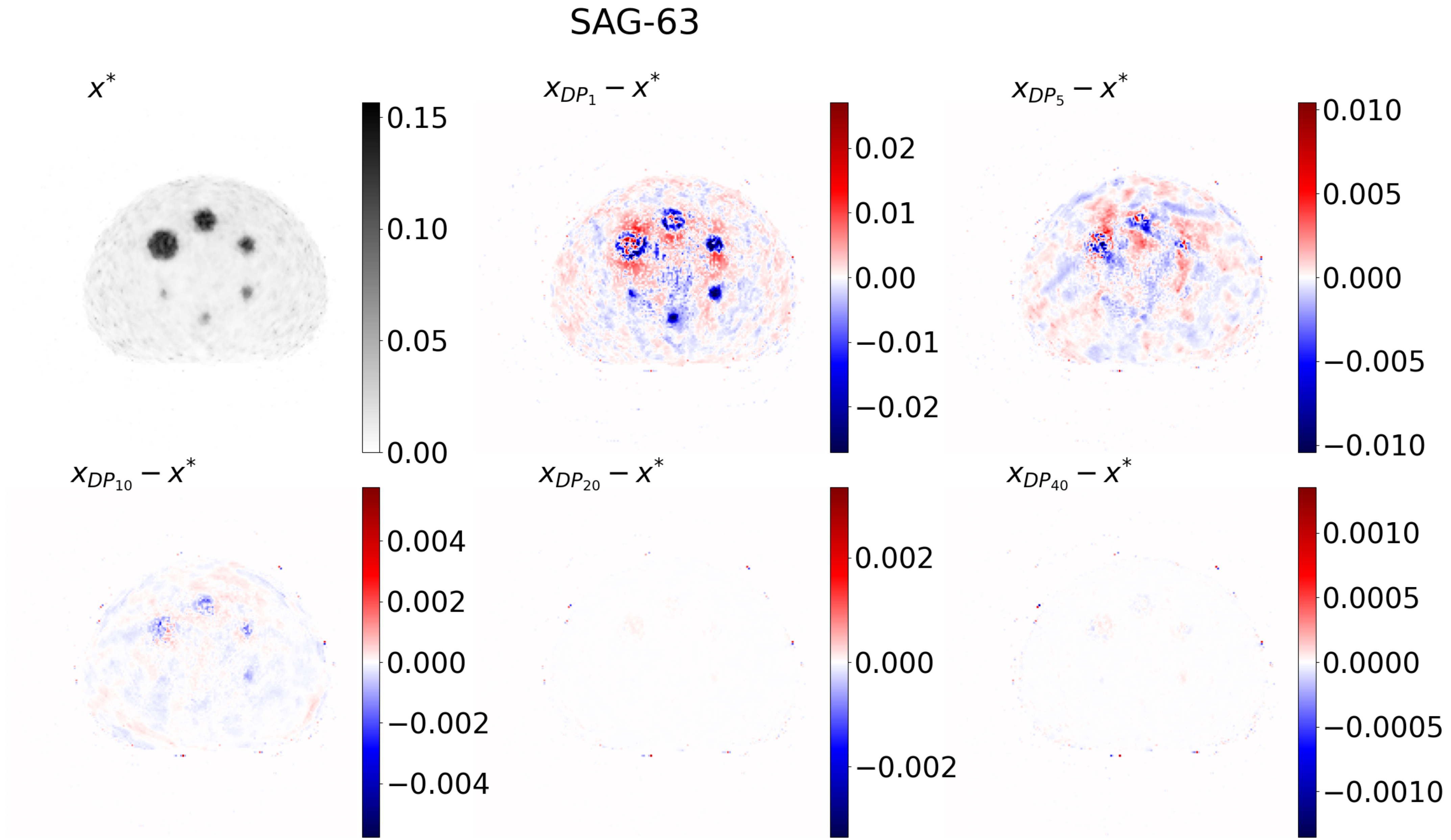
# Applications (PET - Smooth optimisation)



# Applications (PET - Smooth optimisation)



# Applications (PET - Smooth optimisation)



# Summary

- **Stochastic Optimisation Framework in CIL**
- **Flexible and user friendly design with Plug and Play Stochastic Estimators**
- **Different modalities CT, PET, SPECT, MRI**
- **Improvements for CIL Optimisation Module**

- **Website** https://www.ccpi.ac.uk/CIL
- **Docs** https://tomographicimaging.github.io/CIL/nightly/index.html
- **Discord** https://discord.gg/kmBcU2kebB

Thank you for your attention

**https://epapoutsellis.github.io**