Stochastic Optimization of X-ray Micro-CT Domain Size Using PuMA

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Introduction and contextualization

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Importance of porous materials

- **Crucial for the development of Thermal Protection Systems (TPS)**
  - Provides thermal insulation for spacial reentry
  - Re-usable and ablative
- **Ablative TPS**
  - High mechanical stress and temperatures decompose the material (psycho-chemical reactions and erosion)
  - This study deals with transversely isotropic fibrous porous microstructures

Objectives of this study

- Determine the Representative Elementary Volume (REV) of a given porous material using an uncertainty quantification (UQ) methodology
- Discuss the necessary resolution of fibers and digitized domain size to obtain bulk values
- Serve as methodology guideline for future research

Porous Microstructure Analysis (PuMA) software

- Open source software
- Developed at the NASA Ames Research Center under a US & Foreign release
- Can import or artificially generate microstructures
- Perform numerical response simulations
- Able to parallelize computations

https://github.com/nasa/puma

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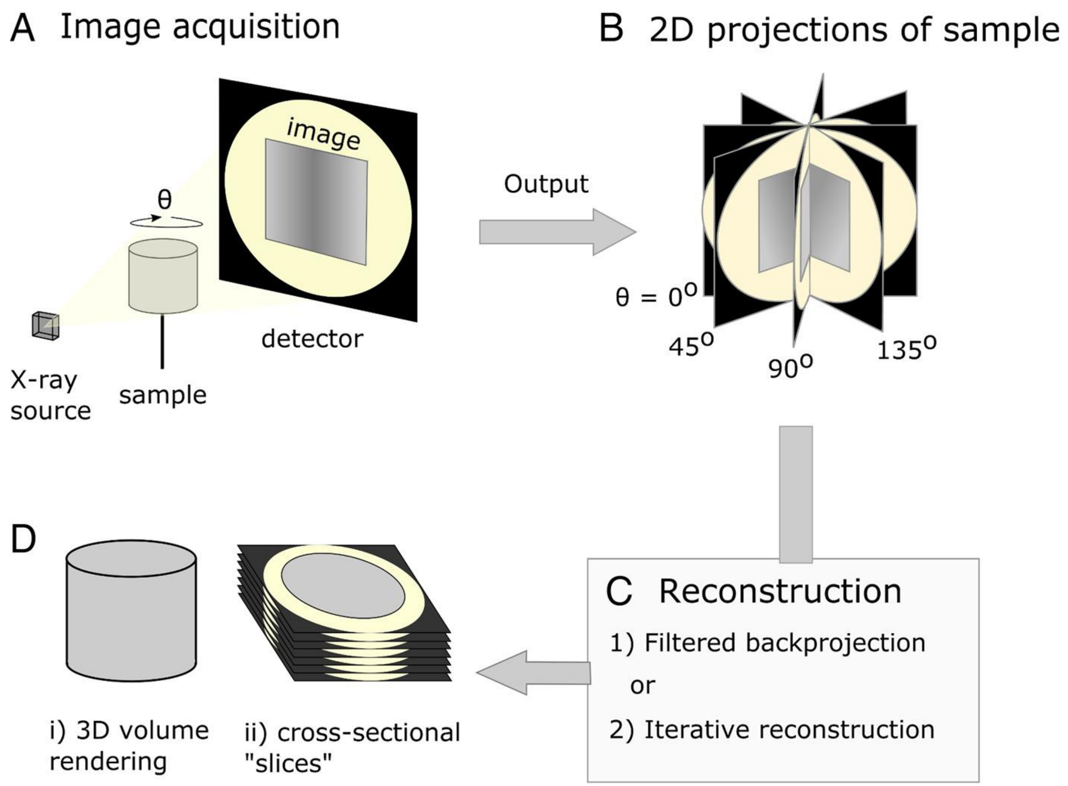
Characterization of Porous Materials Through X-ray Micro-CT

How X-ray microtomography works

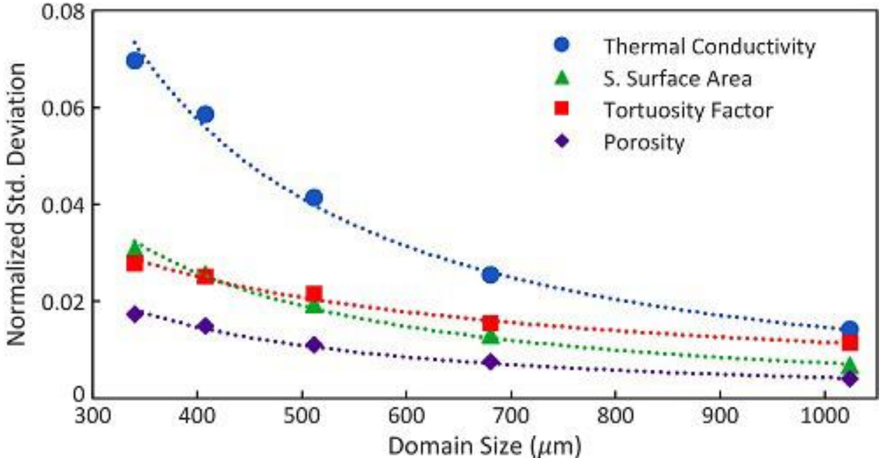
- Pulses of X-ray emitted while the sample is rotating
- Each pulse generates a 2D image, with fixed number of pixels
- 3D model of the sample can be reconstructed by using numerical algorithms



O'Sullivan, James D. B., Julia Behnsen, Tobias Starborg, Andrew S. MacDonald, Alexander T. Phythian-Adams, Kathryn J. Else, Sheena M. Cruickshank, and Philip J. Withers: X-ray micro-computed tomography (ct): an emerging opportunity in parasite imaging. Parasitology, 145(7):848–854, 2018.

Limitations

- Fixed number of voxels for 3D domain
- Trade-off between fiber resolution and physical domain size
  - Conversion between voxels and μm → Voxel Length ℓ_{vx}^{phy}
- Minimal voxel length possible → ℓ_{min}
- Each material property has its own REV for computing bulk property values



Ferguson, Joseph C, Francesco Panerai, Arnaud Borner, and Nagi N Mansour: Puma: The porous microstructure analysis software. SoftwareX, 7:81–87, 2018.

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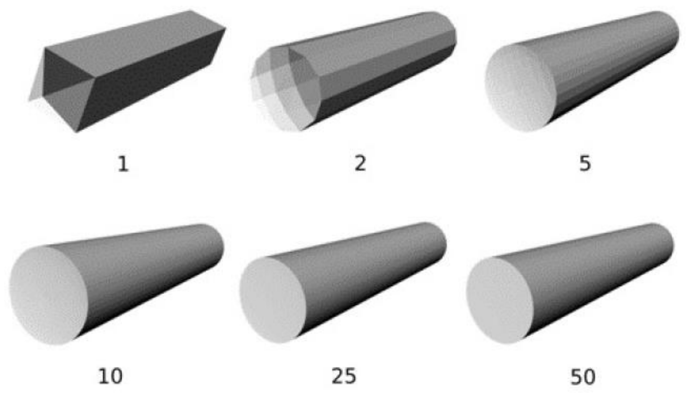
Mathematical formulation of the problem

PuMA wokspace variables

- **Geometrical parameters:**
  - Physical domain length: D_{phy}
  - Average radius of the fiber: R_{phy}
  - Average length of the fiber: L_{phy}
- **Digitized parameters (given in voxels):**
  - Domain length: d_{vx}
  - Average radius of the fiber: r_{vx}
  - Average length of the fiber: l_{vx}
- **Voxel Length:** $\ell_{vx}^{phy} = \dfrac{R_{phy}}{r_{vx}}$



Girault, Florian and Pietro Marco Congedo: Uncertainty Characterization of ablative materials for atmospheric reentry of spacecrafts using PuMA. PhD thesis, Inria Saclay-Île de France, 2021.

PuMA wokspace variables

- **Mechanical properties:**
  - Fiber's thermal conductivity: k_{fiber}
  - Porosity: ε
  - Void phase thermal conductivity: k_{void}
- **Other parameters for generating microstructure:**
  - Angular variation of fibers: $\Delta\theta_i$, where i indicates the direction
  - Standard deviations:
    - $\sigma_{R_{phy}}$ and $\sigma_{L_{phy}}$
  - Solver's tolerance

PuMA wokspace variables

- Relation between D_{phy} and r_{vx}

$$D_{phy} = d_{vx}\ell_{vx}^{phy} = \frac{d_{vx}R_{phy}}{r_{vx}}$$

- X-ray micro-CT limitations on PuMA:
  - $\ell_{vx}^{phy} \geq \ell_{min} \Leftrightarrow r_{vx} \leq r_{max}$
  - $d_{vx} = \text{constant}$
- Trade-off: $D_{phy} \propto \frac{1}{r_{vx}}$
- r_{vx} is the only geometric parameter that will influence the numerical study

Mathematical point of view

- Thermal properties obtained by PuMA: $h(r_{vx}, \xi)$ or $h\left(\ell_{vx}^{phy}, \xi\right)$
  - ξ: Uncertain parameters
- h is stochastic $\longrightarrow$ Compute statistical measures
- Compare results obtained by imposing X-ray micro-CT limitations on PuMA with reference values
- Computation of reference values using the PlaFRIM cluster
  - Greater fiber resolution and domain size than in real micro-CT scans

Mathematical point of view

- **Statistical measures:**
  - $\mu(\cdot)$: Arithmetic mean, or average
  - $Var(\cdot)$: Umbiased estimator of the variance
- **The problem writes as follows:**
  - Minimize: $f_1(k_{ii}) = \left|\mu(k_{ii}) - \mu^{ref}(k_{ii})\right|$
  - Minimize: $f_2(k_{ii}) = \left|Var(k_{ii}) - Var^{ref}(k_{ii})\right|$
  - Satisfying: $\ell_{vx}^{phy} = \frac{R_{phy}}{r_{vx}}$, $\ell_{vx}^{phy} \geq \ell_{min}$, $d_{vx} = \text{constant}$
  - By changing: r_{vx}
- **Search the Pareto-optimal designs in all directions**

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Brute Force Search

Computing the reference values

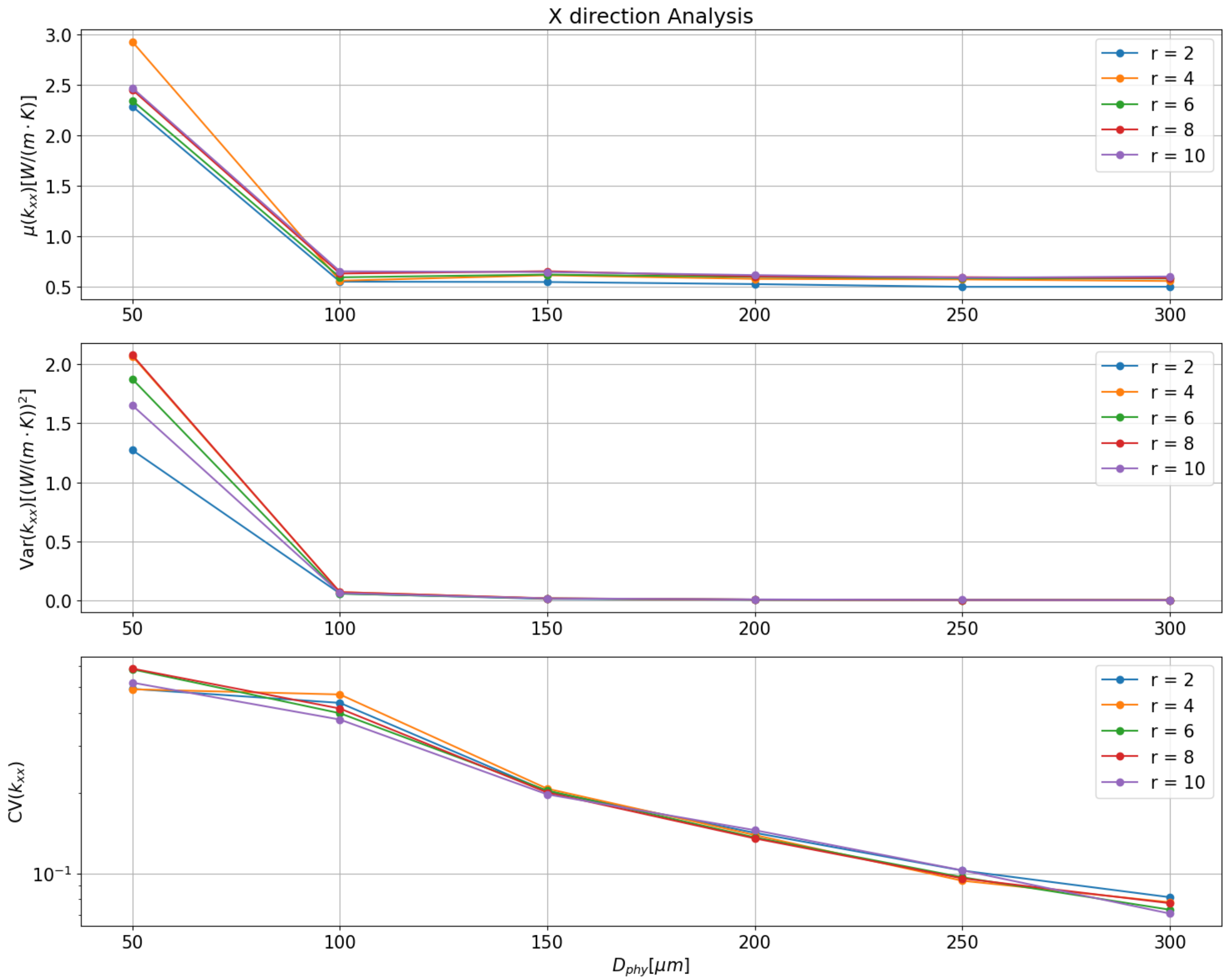
- Fixed input parameters:
  - $R_{phy} = 5\ \mu m$
  - $\sigma_{R_{phy}} = 0.625\ \mu m$
  - $L_{phy} = 800\ \mu m$
  - $\sigma_{L_{phy}} = 500\ \mu m$
  - $\Delta\theta_x = \Delta\theta_y = 90°$
  - $\Delta\theta_z = 20°$
  - $\varepsilon = 0.89$
  - Tolerance $= 1 \times 10^{-4}$
  - $k_{fiber} = 12\ W/(m \cdot K)$

- Fixed thermal conductivity solver options:
  - Explicit-jump finite difference solver
  - Periodic boundary conditions
  - Bi-Conjugate Gradient Stabilized Method for solving linear systems
- This setup is the fastest for generating results

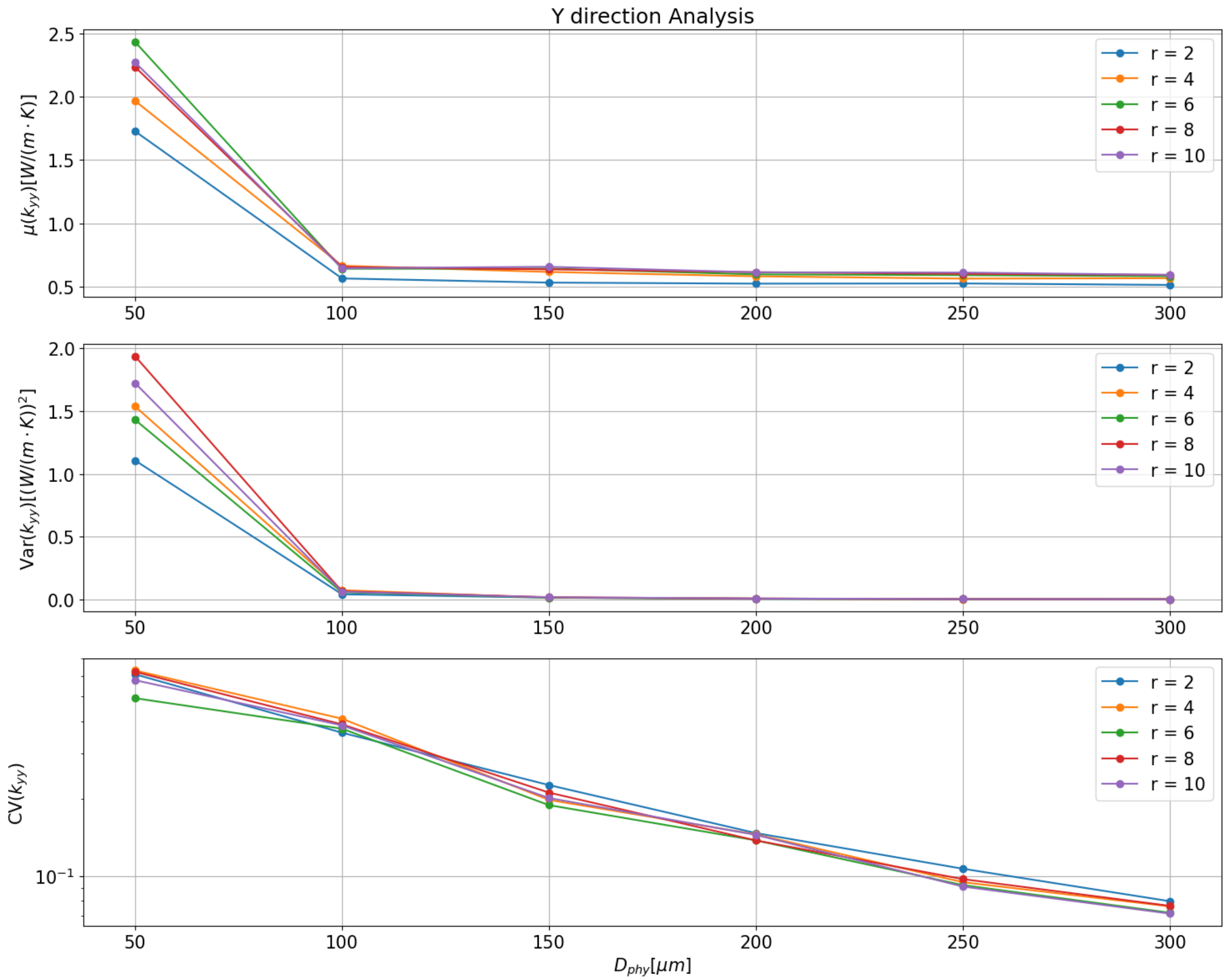
Computing the reference values

- Void phase:
  - $k_{void} = 0.02587\ W/(m \cdot K)$, since this is a proof of concept
- Variable input parameters:
  - $r_{vx} \in \{2,4,6,8,10\}$ voxels
  - $D_{phy} \in \{50,100,150,200,250,300\}\ \mu m$
- Compute thermal conductivities k_{xx}, k_{yy} and k_{zz} for all possible configuration pairs (r_{vx}, D_{phy})
- 1000 simulations per configuration

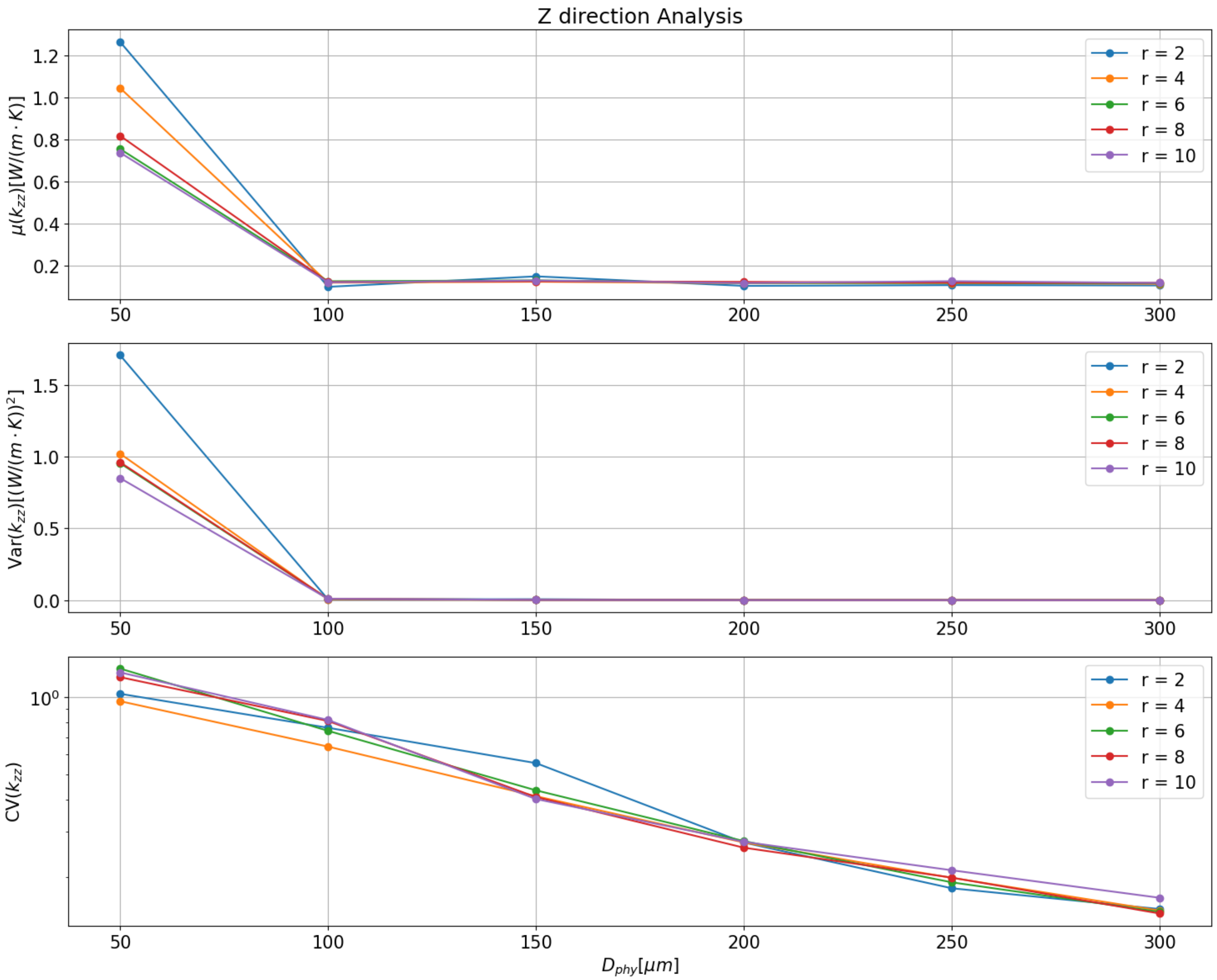
Computing the reference values



Computing the reference values



Computing the reference values



Computing the reference values

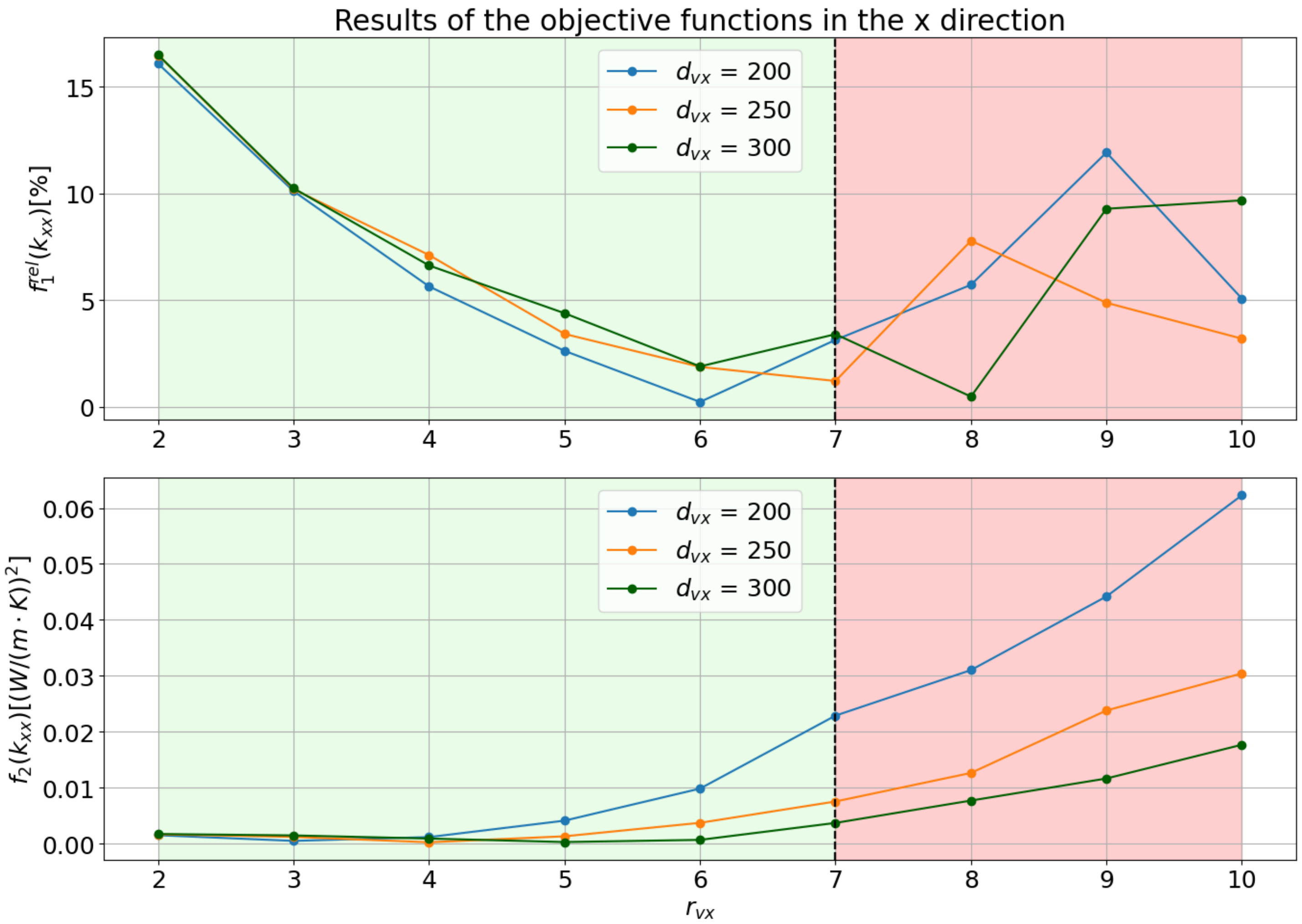
- Results:
  - $\mu^{ref}(k_{xx}) = \ 0.604182\,\mathrm{W/(m \cdot} K)$
  - $\mu^{ref}(k_{xx}) = \ 0.593596\,\mathrm{W/(m \cdot} K)$
  - $\mu^{ref}(k_{xx}) = \ 0.117677\,\mathrm{W/(m \cdot} K)$
  - $Var^{ref}(k_{xx}) = 1.821063 \times 10^{-3}(\mathrm{W/(m \cdot} K))^2$
  - $Var^{ref}(k_{xx}) = 1.789927 \times 10^{-3}(\mathrm{W/(m \cdot} K))^2$
  - $Var^{ref}(k_{xx}) = 3.835413 \times 10^{-4}(\mathrm{W/(m \cdot} K))^2$
- Sidenote: the coefficient of variation (CV) follows exponential behaviour, due to strong linear correlation in log scale

Considering the X-ray micro-CT limitations

- Consider $\ell_{min} = 0.75\,\mu m/\text{voxel} \rightarrow r_{max} = 7$ voxels
- Three different levels of domain resolution:
  - $d_{vx} \in \{200, 250, 300\}$ voxels
- For better visualization of results, consider

$$f_1^{rel}(k_{ii}) = \frac{|\mu(k_{ii}) - \mu^{ref}(k_{ii})|}{\mu^{ref}(k_{ii})}$$

Considering the X-ray micro-CT limitations



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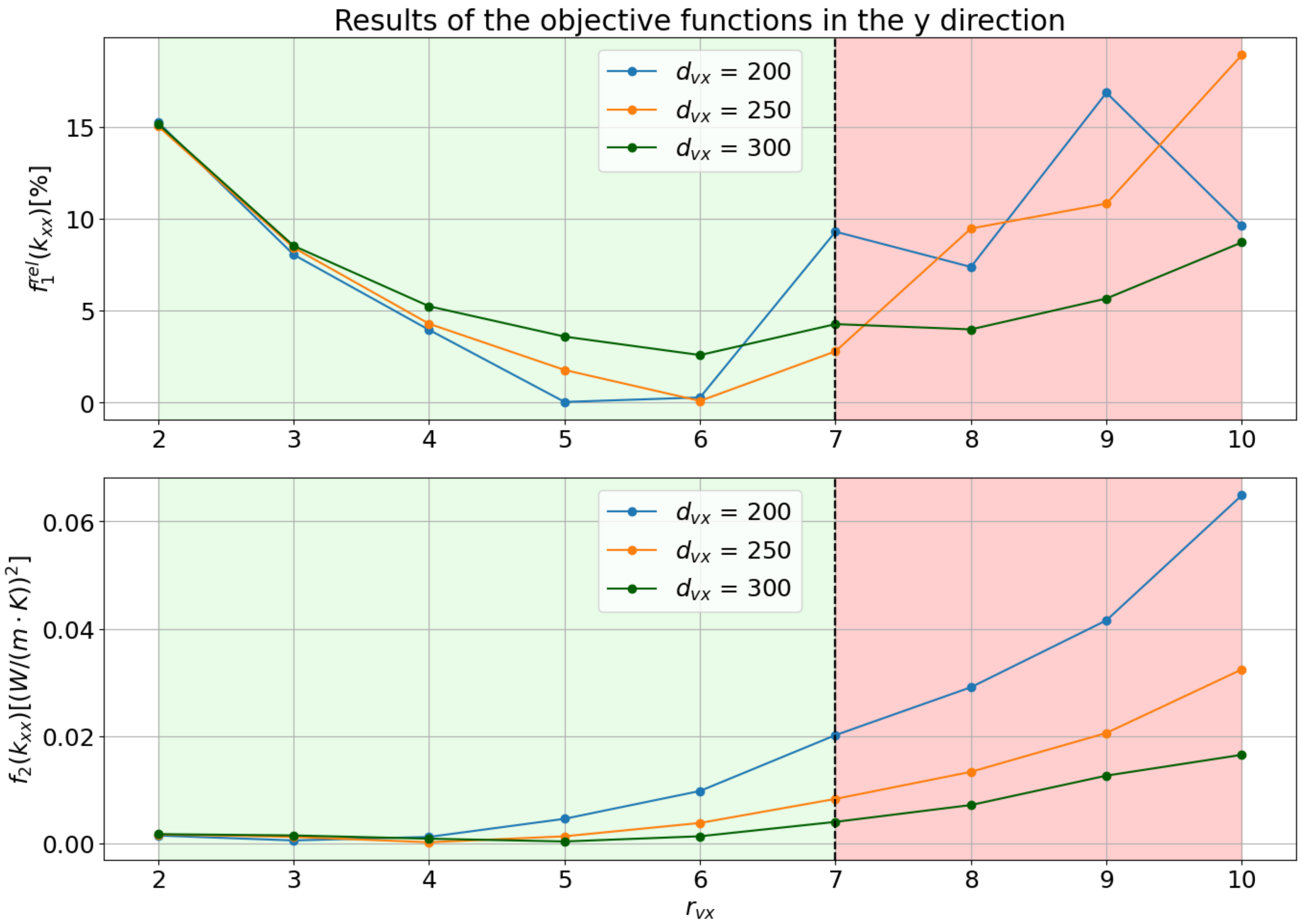

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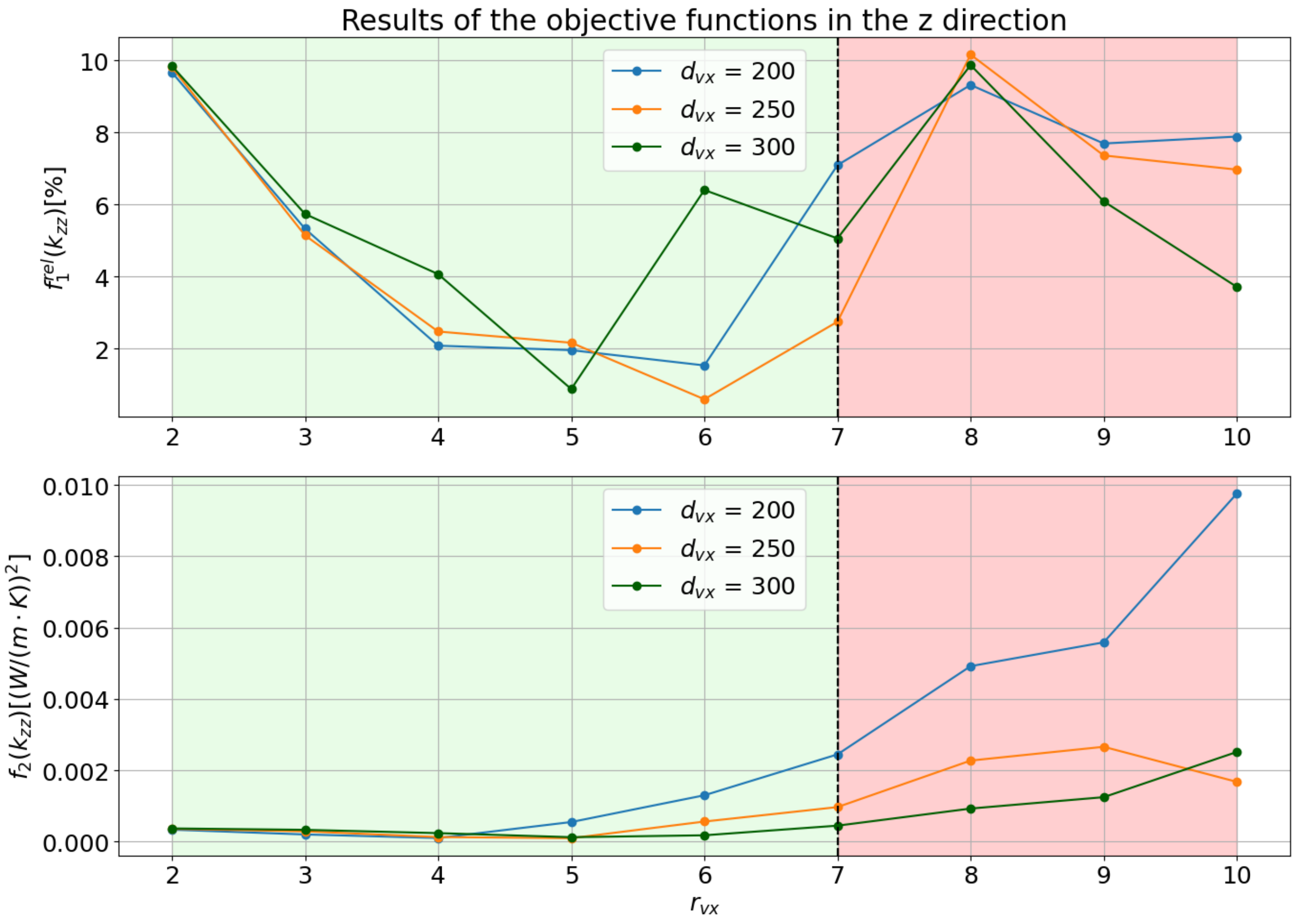
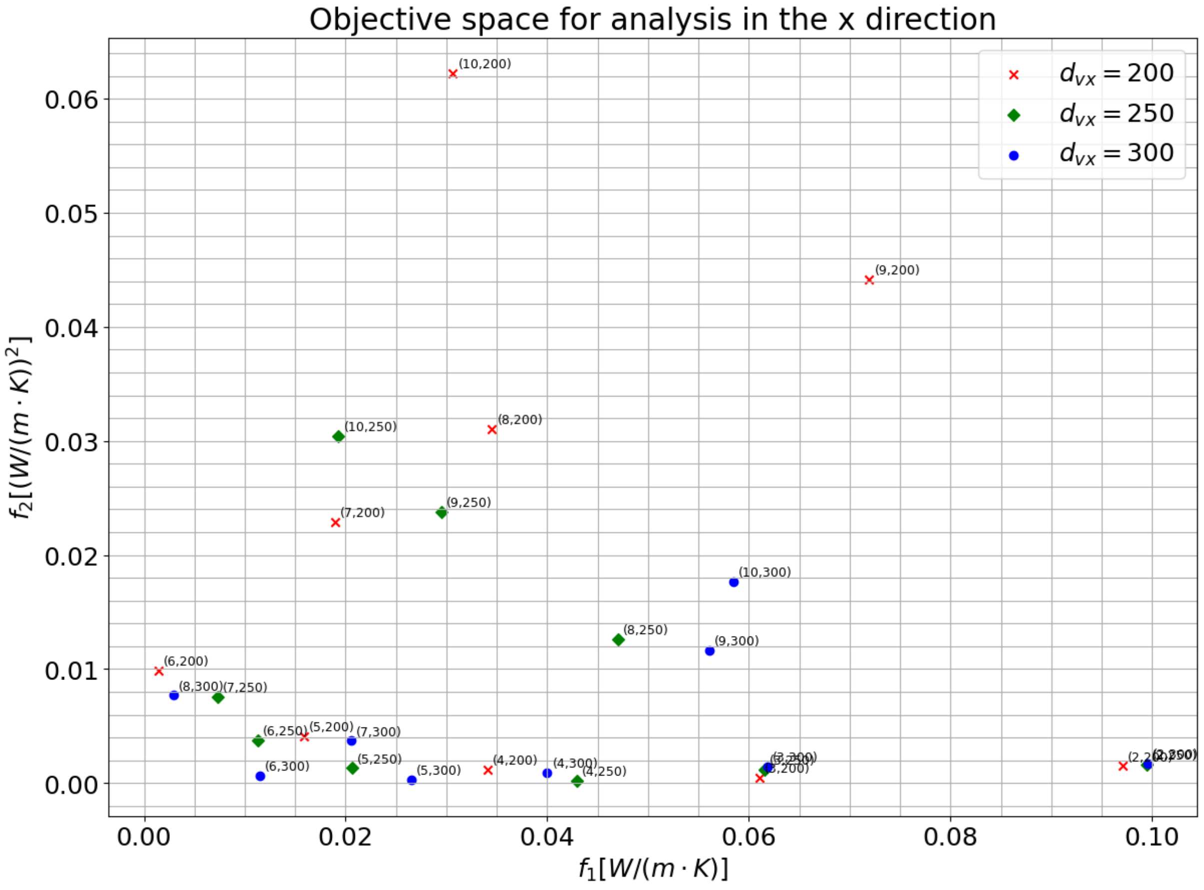


Considering the X-ray micro-CT limitations

- Objective space
  - Search for the pareto front $\mathbb{P}$ in each direction analysis



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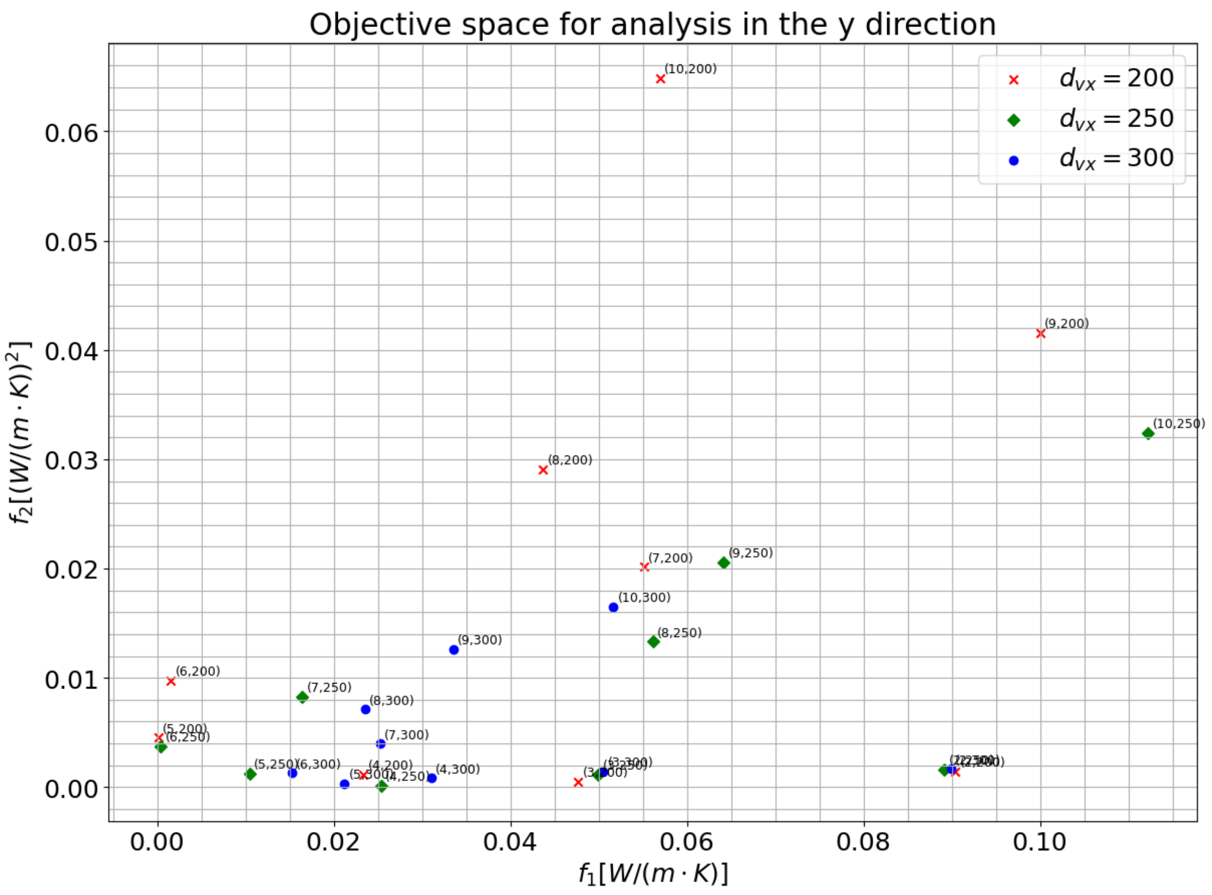


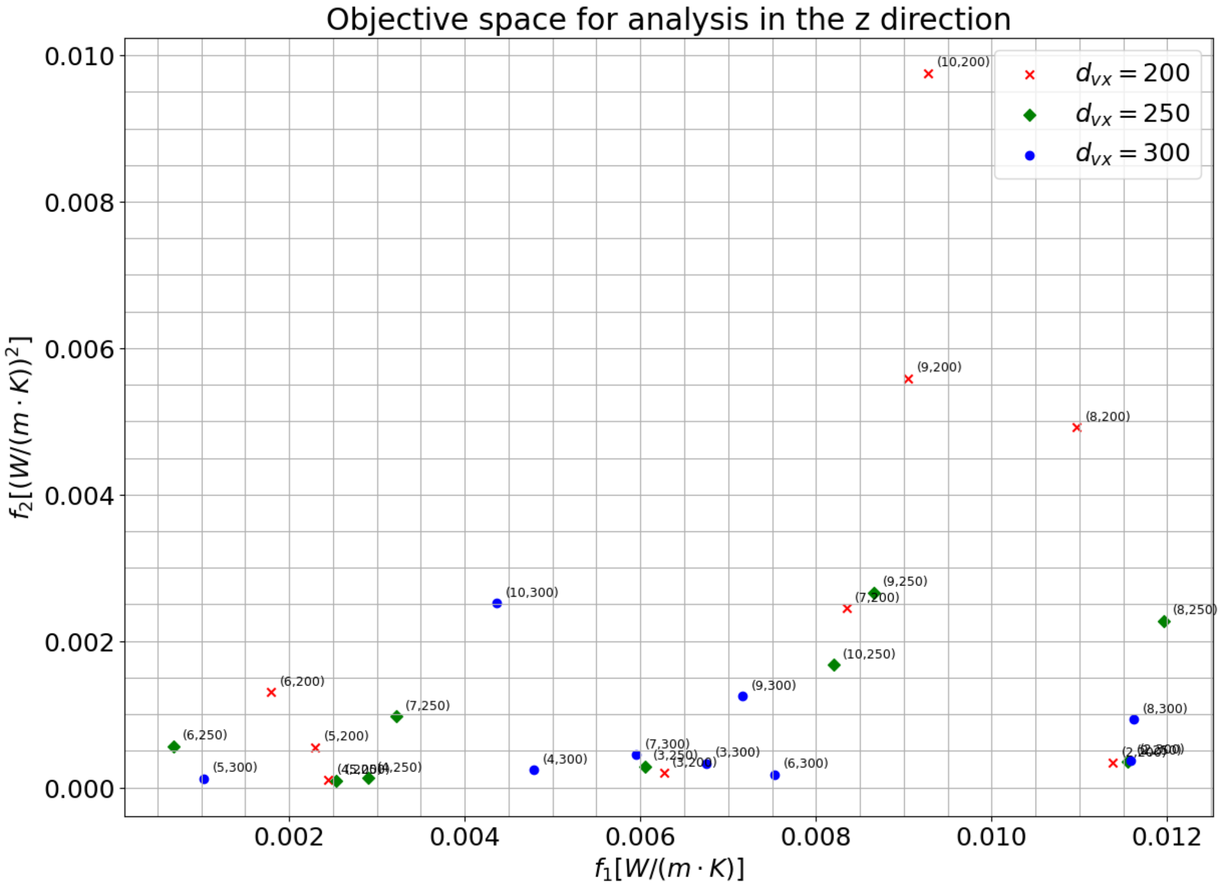
Considering the X-ray micro-CT limitations

- Objective space
  - Search for the pareto front $\mathbb{P}$ in each direction analysis

Pareto front

d_{vx}	$\mathbb{P}_x(X)$	$\mathbb{P}_y(X)$	$\mathbb{P}_z(X)$
200	{3,4,5,6}	{3,4,5}	{4,5,6}
250	{4,5,6,7}	{4,5,6}	{5,6}
300	{5,6,8}	{5,6}	{5}

Value dismissed, since $r_{max} = 7$ voxels



Computing the optimal values of D_{phy}

- **Estimation of optimal D_{phy}:**
  1) Obtain range of D_{phy} values for a given direction and d_{vx} value
  2) Average out the limits of this range → D_{phy}^{avg}
  3) Compute arithmetic mean of these averages, considering all d_{vx} values
- **Results:**
  - $\left(D_{phy}^{opt}\right)_x = 256.85\ \mu m$
  - $\left(D_{phy}^{opt}\right)_y = 267.36\ \mu m$
  - $\left(D_{phy}^{opt}\right)_z = 245.83\ \mu m$

$$\xrightarrow{\text{Average}} D_{phy}^{opt} = 256.52\ \mu m$$

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The SAMATA Algorithm

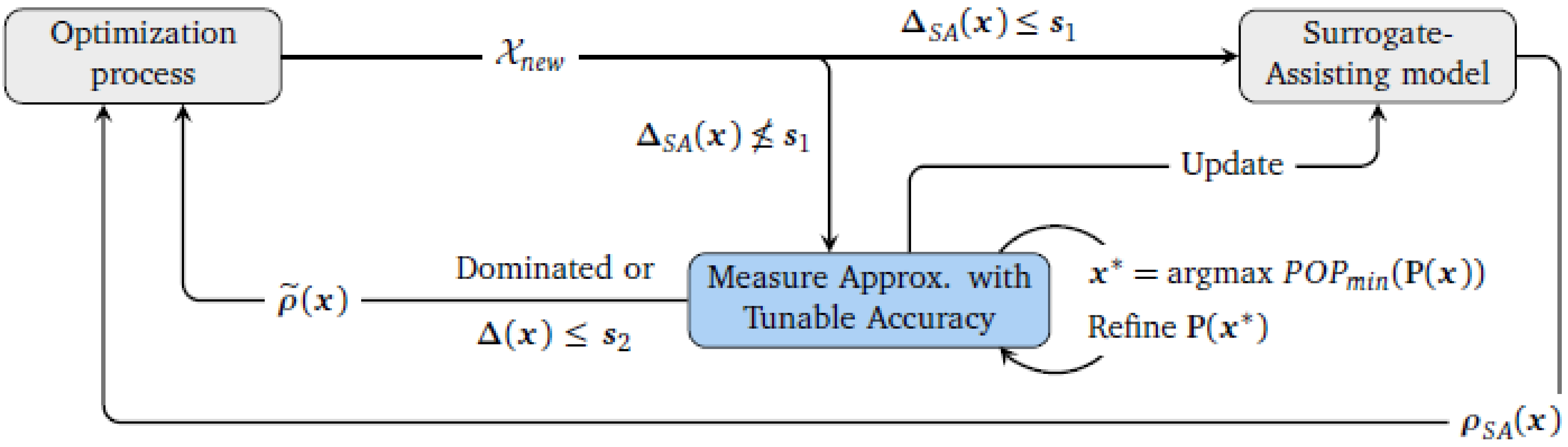
Brief introduction to the algorithm

- Will explore the formulated problem with a probabilistic optimization framework
- Objective functions → Robustness measures ρ_f
- ρ_f will be a statistical measure and considered as random vector from a random field $\boldsymbol{P}$
- Advantages of using SAMATA:
  - Algorithm prioritizes computational power to most promising designs
    - Rank designs → Pareto-optimal probability (POP)
  - Reduces the number of computations and designs to obtain optimal results

Brief introduction to the algorithm

- SAMATA relies on
  - Measure Approximation with Tunable Accuracy (MATA)
  - Surrogate-assisting model (SA)
- The MATA approach is designed to tune the accuracy of each computation of statistical measures ρ
  - Focus computational power on the best designs
- The SA strategy is designed to give predictions for robustness measures
  - Relies on heteroscedastic Gaussian Processes and Kernel Density Estimation (KDE) strategy
- Two used-defined thresholds to control the optimization process: s_1 and s_2

Brief introduction to the algorithm



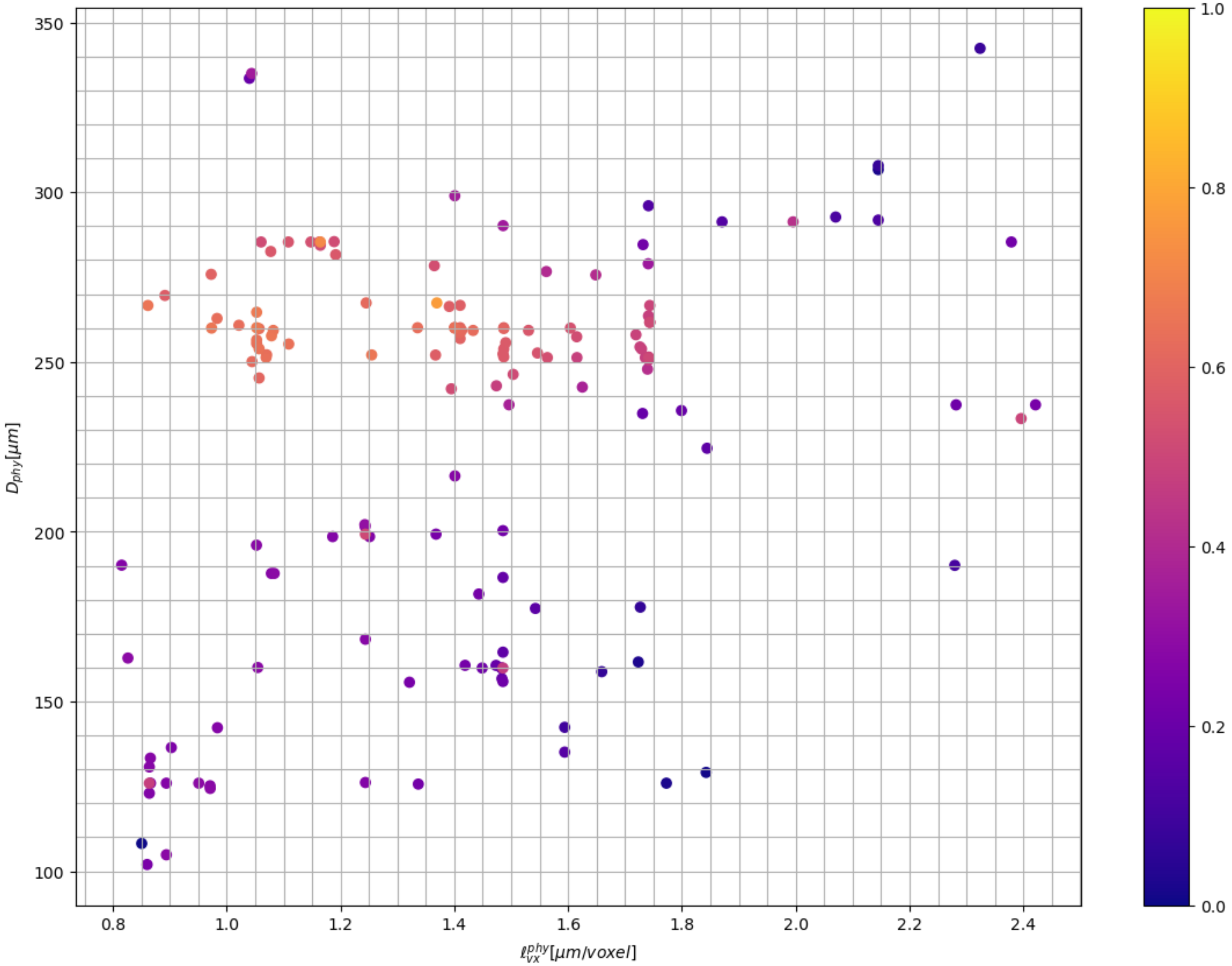
Rivier, Mickael: Low-cost methods for constrained multi-objective optimization under uncertainty. PhD thesis, Institut Polytechnique de Paris, 2020.

Results using SAMATA

- **New formulation:**
  - Minimize: $f_1(k_{zz}) = \left|\mu(k_{zz}) - \mu^{ref}(k_{zz})\right|$
  - Minimize: $f_2(k_{zz}) = \left|Var(k_{zz}) - Var^{ref}(k_{zz})\right|$
  - By changing: $\left(D_{phy}, \ell_{vx}^{phy}\right) \in [100,350] \times [0.75,2.5]$
- **SAMATA thresholds:**
  - s_1 and s_2 equal and belonging to $\{1,0.8,0.6,0.4\}$
  - Decreased values are used to avoid bias introduced by an empirical choice of one threshold

Results using SAMATA

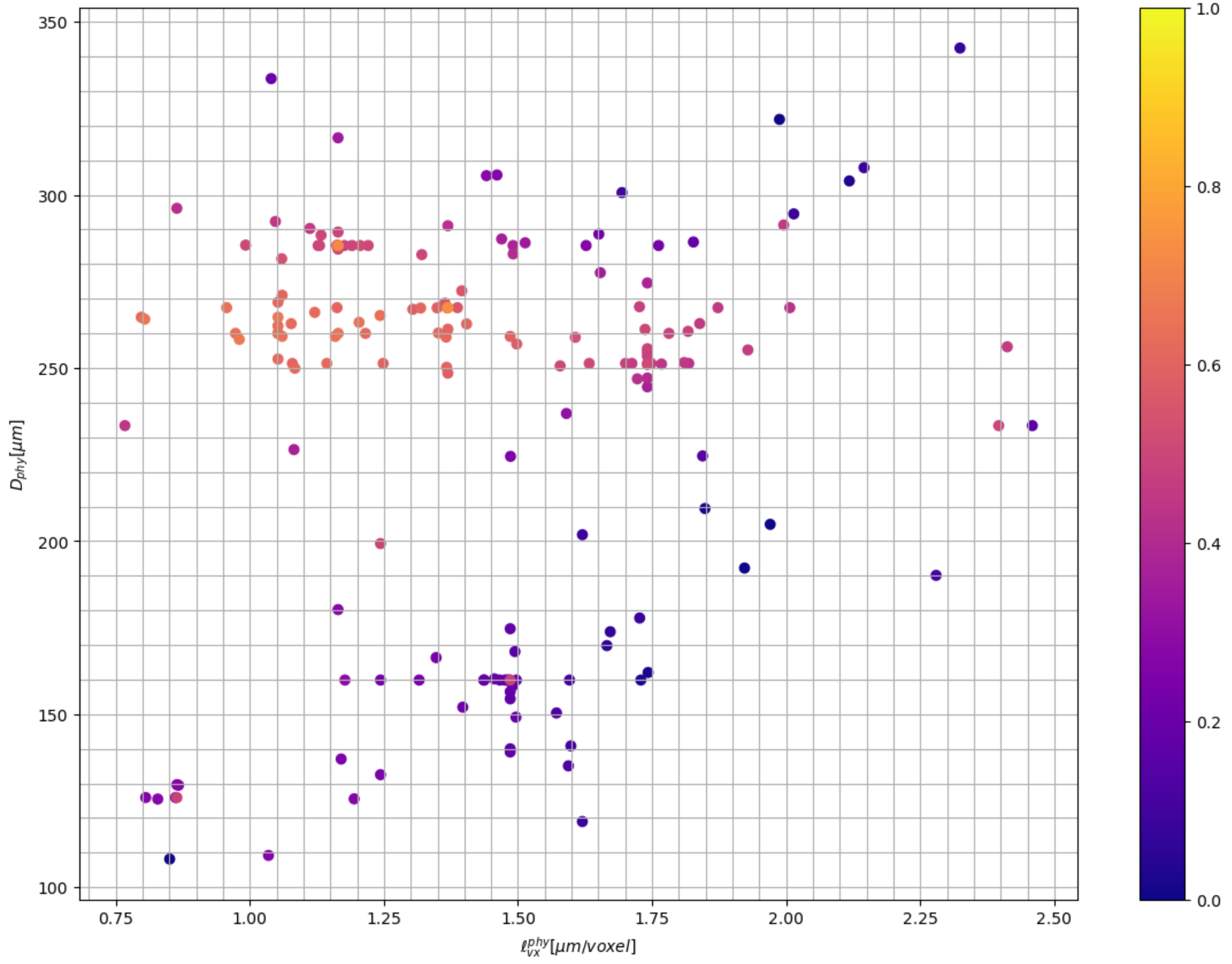
1) $s_1 = s_2 = 1$



Results using SAMATA

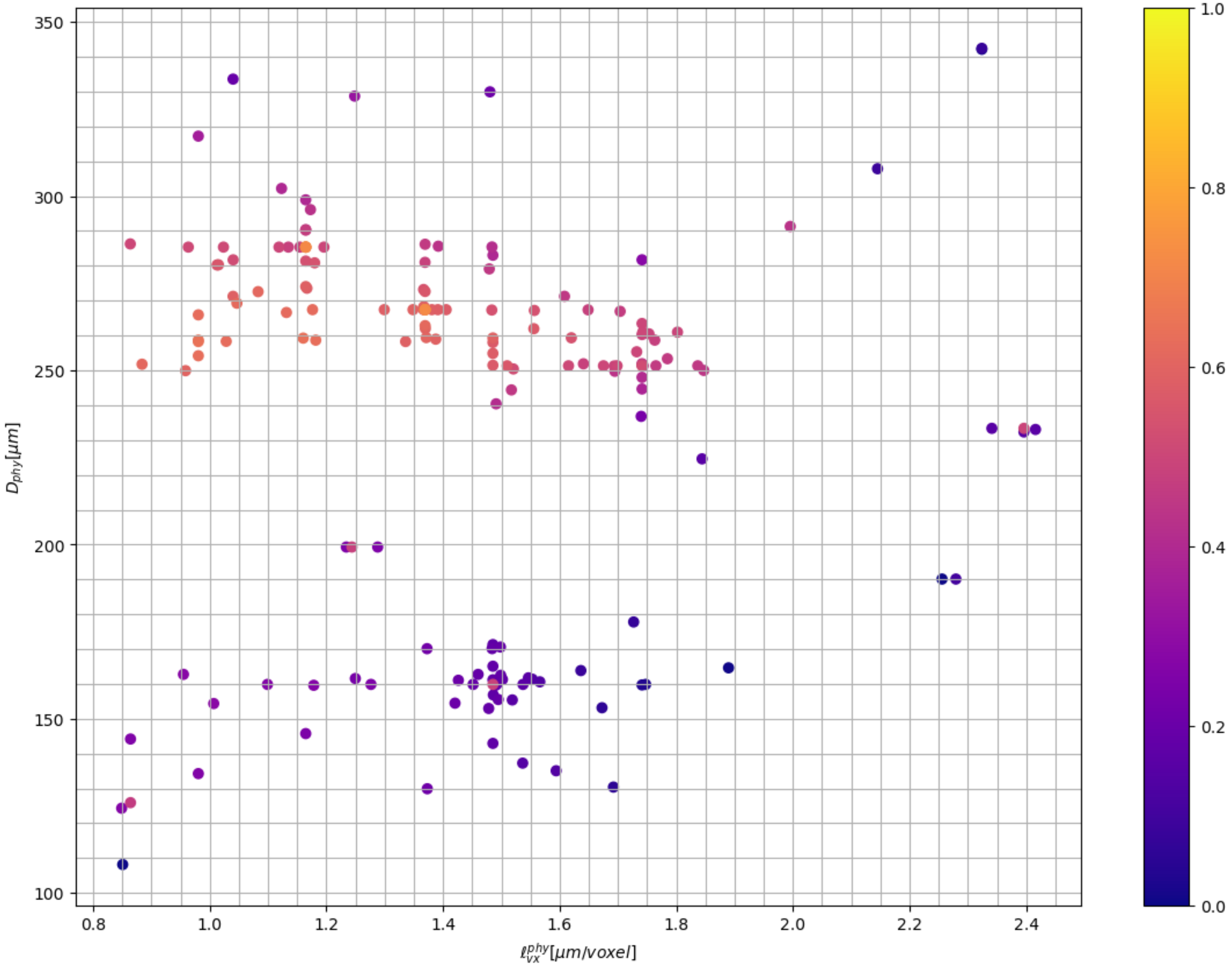
1) $s_1 = s_2 = 1$

2) $s_1 = s_2 = 0.8$



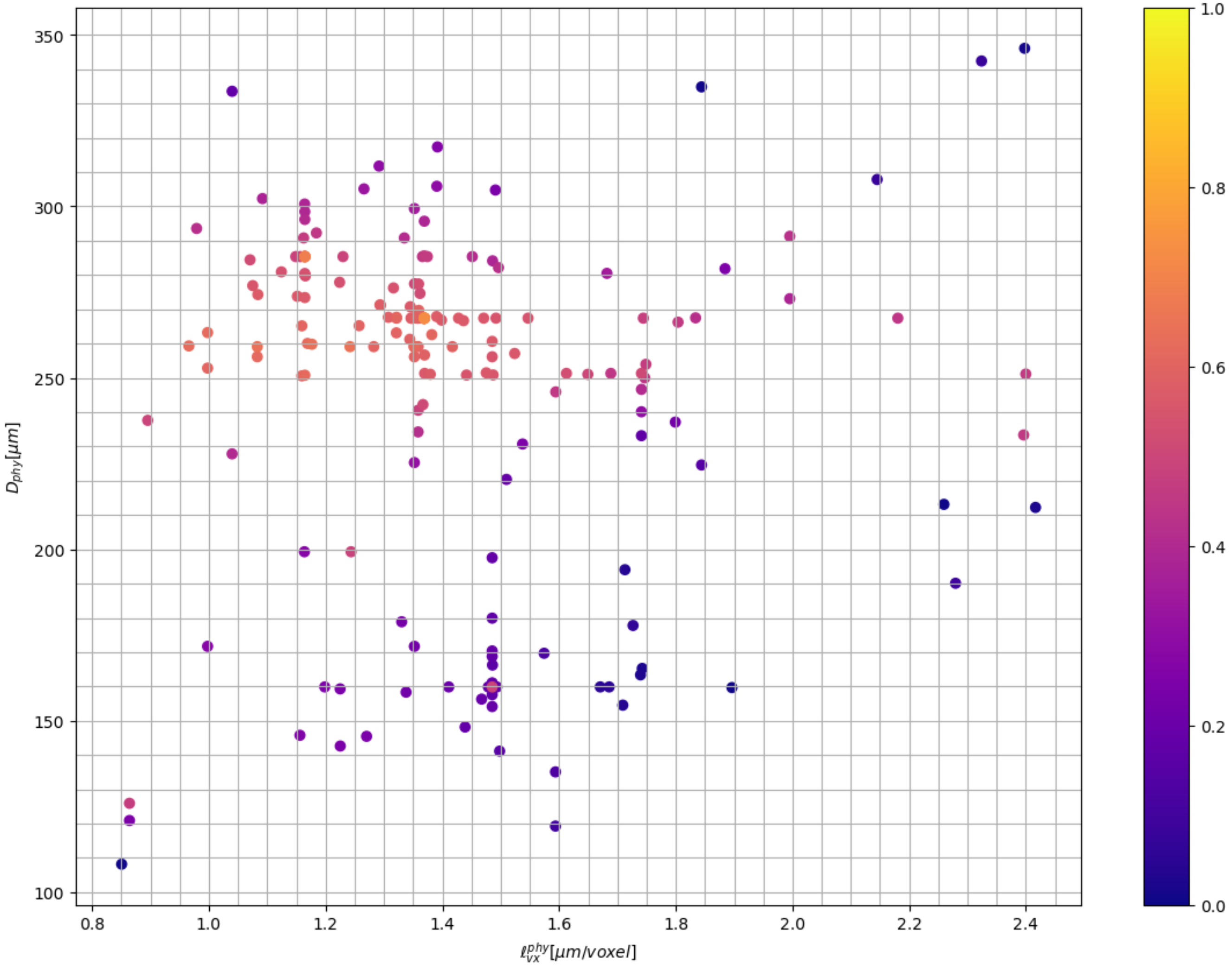
Results using SAMATA

1) $s_1 = s_2 = 1$
2) $s_1 = s_2 = 0.8$
3) $s_1 = s_2 = 0.6$



Results using SAMATA

1) $s_1 = s_2 = 1$
2) $s_1 = s_2 = 0.8$
3) $s_1 = s_2 = 0.6$
4) $s_1 = s_2 = 0.4$



Results using SAMATA

- Optimal results falls within a band of values
  - $D_{phy} \in [250{,}270]\ \mu m$
- Results close to the ones obtained by brute force
- More reliable analysis
- Reduction of approximately 90% in the number of needed simulations on PuMA
- Demonstrates that the REV is not dependent on d_{vx} of the machine
- Algorithm can analyse multiple machine powers at the same time, by letting d_{vx} free

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Conclusion

Conclusion

- This study provides a general guideline for coupling the UQ framework with PuMA
- PuMA demonstrates to have a huge potential for helping researchers in the aerospace field
- Having higher fiber resolution does not imply in having better results
- The probabilistic framework gave us a more reliability, together with reduction in time and costs
- The results obtained are strongly dependent on the reference values computed
- Further study can be done with latest version of PuMA

Thank you for your attention!

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