

Software for the Practical Analysis of Materials

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ISRD-RCN Workshop: "Exploring Dynamic Properties of Earth and Planetary Materials Using Neutron and X-Ray Methods"

Grenoble, 23/05/2024



Let's play with some images

General information

What is Span ?



python library



(with some bits of C++)





(with some bits of C++)

(not AI enhanced!)





(with some bits of C++)

(not AI enhanced!)

X-ray & Neutron tomography (for example)





(for example)

Strictly open-source !

Why do we need a software like Spain?





Why do we need a software like Spanner?



Sandstone



MORPHOLOGY

- Phase identification
- Volume fractions
- Size, shape
- Orientation, fabric
- Tortuosity, connectivity

Why do we need a software like Spanna ?

$\operatorname{Concrete}$





Sandstone



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Lentils



Sandstone



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Why do we need a software like Span





- δ (Volume fractions)
- δ (Size, shape)
- δ (Orientation, fabric)
- δ (Tortuosity, connectivity)
- KINEMATIC FIELDS

Why do we need a software like Span ?

Concrete displacement field



[Stamati O. (2021) Cem. Concr. Research]





[Pinzón G. (2023) Gran. Matter]

- $-\delta$ (Volume fractions)
 - $-\delta$ (Size, shape)
 - δ (Orientation, fabric)
 - δ (Tortuosity, connectivity)
 - KINEMATIC FIELDS

Flow in sandstone



[Couture C. (in preparation)]



Examples of measuring deforming media with

Concrete fracture



[Stamati O. (2021) Cem. Concr. Res.]

Particle tracking



[Pinzón G. (2023) Gran. Matter]



Sandstone failure



[Cartwright-Taylor A. (2022) Nature Comm.]

Claystone water absorption



[Stavropoulou E. (2020) Front. in Earth Science]

Tendon/Bone Interface



[Sensini A. (in preparation)

Let's play with some images









y([[3317		29859,	31265, 2	28414,	30618,	31769,	σ,	υ,	σ,	
1624	11,	29112,	29486],							
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1064,	0,	29666],					
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Binarised image







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Particle volumes image









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Particle volumes image

S example: Morphological measurements

```
# import modules
1
    import numpy. tifffile
2
    import spam.label, spam.plotting
3
4
    # 1. load image and plot the grey level histogram
5
    im = tifffile.imread("grains.tif")
6
     spam.plotting.plotGreyLevelHistogram(grey, showGraph=True)
7
8
    # 2. identification of grains
    binary = im >= 18000
9
10
     # 3. labelling of grains
    labelled = spam.label.watershed(binary)
11
    # 4. volumes calculation
12
     volumes = spam.label.volumes(labelled)
13
     plt.hist(volumes, bins=64); plt.xlabel("Volume (vx)"); plt.ylabel("count"); plt.show()
14
    # 5. plot particle size distribution
15
    radii = spam.label.equivalentRadii(labelled)
16
     spam.plotting.plotParticleSizeDistribution(radii*15*4/1000.0, bins=256, units="mm")
17
     # 6. visualise the grains coloured with volumes
18
19
    labelledMaxVol = spam.label.convertLabelToFloat(labelled, volumes)
    plt.imshow(labelledMaxVol[:, :, labelledMaxVol.shape[2]//2], cmap="plasma"): plt.show()
20
```

E^{Read} https://www.spam-project.dev/docs/tutorials/tutorial-03-labelToolkit.html







9

image 1	image 2	residual
array([[11931, 11145, 11508, 12270, 12040, 12514, 13176, 14835, 20326, 29225, 34191, 21655, 12285],	array([[32738, 28492, 14357, 9786, 9831, 10480, 15689, 17897, 1505 11978, 11473, 11169, 11038],	
[18759, 12223, 12034, 12864, 13021, 12939, 12926, 16789, 23822, 29928, 33987, 26894, 13810],	[27755, 21958, 12138, 10322, 10209, 9708, 12119, 16130, 1593 13200, 12479, 11724, 11014],	3,
[27971, 15814, 12261, 12486, 13352, 12963, 12321, 17037, 25474, 31316, 33720, 31330, 17174],	[16983, 12342, 10224, 10482, 11079, 10295, 11008, 14399, 1631 14135, 12619, 11464, 10691],	
[30987, 18643, 12490, 13615, 13259, 12608, 12316, 17200, 26466, 31433, 32565, 32627, 245291.	[10408, 9032, 9688, 11002, 11866, 10993, 11439, 12952, 1598 16938, 19381, 21616, 19468].	[0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0
[30940, 20799, 13864, 13810, 12368, 12428, 12638, 14913, 22127,	[10976, 10456, 9832, 9996, 10933, 11927, 11476, 11817, 1396	6, [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
[30308, 20819, 13442, 13171, 12174, 11788, 13367, 15867, 18360,	[11100, 10816, 10411, 10206, 10400, 10965, 11633, 12334, 1273	2, [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
20400, 23084, 24087, 21327], [28231, 16996, 12774, 11774, 10907, 11451, 17046, 24109, 26307.	19483, 29714, 31859, 30801], [17810, 11712, 10137, 10624, 11086, 10827, 11452, 11589, 1165	
18931, 12581, 12947, 11612],	16397, 26023, 29611, 26193],	
[20042, 11917, 12057, 11458, 10142, 12744, 21917, 30117, 32083, 26414, 13083, 9227, 9560].	[32045, 20023, 17541, 11582, 11310, 12237, 12102, 12005, 1140 12752, 18506, 20914, 16539].	³ , [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
[11830, 10643, 11377, 11326, 9810, 12978, 24110, 30924, 32738,	[33943, 33966, 32197, 21946, 11953, 13484, 13231, 13101, 1243	3, [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
28492, 14357, 9786, 9831], [10034, 10527, 11255, 11807, 10928, 11390, 18715, 25353, 27755,	[33859, 32898, 34371, 32940, 16905, 12897, 13213, 12454, 1271	
21958, 12138, 10322, 10209],	12339, 12456, 13448, 13074], [13059, 22042, 23507, 24144, 24247, 12724, 12244, 11712, 1152	[0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]], dtype=uint16)
12342, 10224, 10402, 11079],	12905, 13032, 13041, 12610],	
[10336, 9713, 11265, 12484, 11966, 11322, 11061, 10848, 10408,	[32681, 32889, 32693, 34115, 25019, 12476, 12798, 10718, 1111 12560, 12914, 12959, 11956]	1,
[13713, 11569, 12586, 13535, 11586, 10646, 10546, 10882, 10976,	[26569, 32452, 33644, 31245, 17666, 11383, 12677, 11976, 1187	٥,
10456, 9832, 9996, 10933]], dtype=uint16)	12189, 12612, 12771, 11369]], dtype=uint16)	

The general idea of Digital Volume Correlation (DVC)

DVC aims to find a **transformation** that links two 3D images f(x) and g(x).

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 $f(\boldsymbol{x}) - g(\boldsymbol{\Phi} \cdot \boldsymbol{x}) = 0$

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Deformation function in Space $\boldsymbol{\Phi} = \left| \begin{array}{cccc} F_{zz} & F_{zy} & F_{zx} & t_z \\ F_{yz} & F_{yy} & F_{yx} & t_y \\ F_{xz} & F_{xy} & F_{xx} & t_x \\ 0 & 0 & 0 & 1 \end{array} \right| \quad \text{with} \quad \boldsymbol{x} = \left(\begin{array}{c} z \\ y \\ x \\ 1 \end{array} \right) \quad \text{and} \quad \boldsymbol{x}' = \boldsymbol{\Phi} \cdot \boldsymbol{x}$ where Φ is **linear** and **homogeneous** accounting for: translation, rotation, normal and shear strain

The general idea of Digital Volume Correlation (DVC) in Spam

Gradually **minimise** the SSD between the **reference** image f and the **deformed** image \tilde{g} corrected by a **trial** deformation function $\tilde{\Phi}$:

$$\mathcal{T}(\widetilde{\Phi}) = \frac{1}{2} \sum_{\boldsymbol{x} \in \Omega} \left(f(\boldsymbol{x}) - g(\widetilde{\Phi} \cdot \boldsymbol{x}) \right)^2 \text{ with } \Phi = \operatorname*{argmin}_{\widetilde{\Phi}} \mathcal{T}(\widetilde{\Phi})$$

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A Gauss-Newton iterative scheme is implemented based on a 1st order Taylor expansion of the updated deformed image \tilde{g} for small corrections of $\delta \Phi$:

$$g(\boldsymbol{\Phi}^{(n+1)} \cdot \boldsymbol{x}) = g(\boldsymbol{\Phi}^{(n)} \cdot \boldsymbol{x}) + \boldsymbol{\nabla} g(\boldsymbol{\Phi}^{(n)} \cdot \boldsymbol{x}) \cdot \delta \boldsymbol{\Phi}^{(n+1)} \cdot \boldsymbol{\Phi}^{(n)} \cdot \boldsymbol{x}$$
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The system in a matrix-vector format:

$$M^{(n)}\delta\Phi^{(n+1)} = A^{(n)}$$

- M is the Hessian: gradient of g and
- ${\boldsymbol A}$ is the Jacobian: contains the difference between f and \widetilde{g}



 $g({m x})$







initial Φ

 $g(\boldsymbol{x})$



initial difference



 $g(\Phi \cdot \boldsymbol{x})$





 $g(\boldsymbol{x})$







initial difference































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Correlation windows defined on a regular grid

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Displacement field

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Correlation windows defined on a regular grid





Correlation windows defined on labels

Hall S. et al.: Discrete and continuum experimental study of localised deformation in hostun sand under triaxial compression using x-ray ct and 3d digital image correlation, Géotechnique (2010)

Andò E. et al.: Experimental micromechanics: grain-scale observation of sand deformation, Géotechnique Letters (2012)

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How to produce these deformation fields with

1. Initial registration script called from bash

1	bash> spam-register	#	The	script for the	initial	alingment
2	01.tif 02.tif	#	The	two tiff files	to load	

2. Regular grid DVC script called from bash

1	bash> spam-ldic	#	The script for the structured grid
2	01.tif 02.tif \	#	The two tiff files to load
3	-pf 01-02-registration.tsv \	#	Initial guess from the script above
4	-hws X \	#	Half-size of the correlation window
5	-ns X \	#	The node spacing of the grid
6	-tsv -vtk -tif	#	Ask for TSV, TIFF and VTK file outputs

3. Strains script called from bash

```
      1
      bash> spam-regularStrains
      # The script for the structured strains

      2
      01-02-ldic.tsv \
      # Deformation field from the script above

      3
      -tsv -vtk -tif
      # Ask for TSV, TIFF and VTK file outputs
```

How to get a deformation field through time?

DVC on a regular grid



[Stamati O. (2021) Cem. Concr. Res.]

DVC on labelled objects



[Pinzón G. (2023) Gran. Matter]

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[Pinzón G. (2023) Gran. Matter]

Both are considered as local correlation approaches

Global vs Local DVC approaches

The paradigm behind the global correlation is to transform an image with a displacement field which support is a Finite Element mesh instead of a set of linear operators Φ .



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Global vs Local DVC approaches

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Hild F. and Roux S.: Comparison of local and global approaches to digital image correlation, Experimental Mechanics (2012)

A Finite Element mesh to transform an image

The global DVC problem can be expressed as the following functional to minimize:

$$\Phi_{ ext{c}} = \sum_{\Omega} \|g(oldsymbol{x} + oldsymbol{u}(oldsymbol{x})) - f(oldsymbol{x})\|_2$$

where:

• u(x) = N(x)d is the displacement field supported but standard FE shape functions

A Finite Element mesh to transform an image

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In it's weak form can be solved with a Newton-Raphson method:

$$M_c \delta d = b$$

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$$\boldsymbol{M}_c \delta \boldsymbol{d} = \boldsymbol{b}$$

where:

- u(x) = N(x)d is the displacement field supported but standard FE shape functions
- + δd is the increment of displacement field unknowns d
- M_c can be seen as a FE assembled mass matrix
- \boldsymbol{b} contains the residual supported by the shape functions

Mechanically driven Tikhonov regularization

Equilibrium gap method: Minimizing the distance between current solution u and that which satisfies the equation for linear elasticity.

$$\left\{ egin{array}{ll} \Phi_{\mathrm{c}}(oldsymbol{d}) = \sum_{\Omega} \|g(oldsymbol{x}+oldsymbol{u}(oldsymbol{x})) - f(oldsymbol{x})\|_2
ight.$$

The regularised problem becomes:

 $(\boldsymbol{M}_{c} + \boldsymbol{M}_{\mathrm{reg}}) \, \delta \boldsymbol{d} = \boldsymbol{b} - \boldsymbol{M}_{\mathrm{reg}} \boldsymbol{d}$

Mendoza A., Neggers J., Hild F., Roux S.: Complete mechanical regularization applied to digital image and volume correlation, Computer Methods in Applied Mechanics and Engineering (2019)

Mechanically driven Tikhonov regularization

Equilibrium gap method: Minimizing the distance between current solution u and that which satisfies the equation for linear elasticity.

$$egin{aligned} & \Phi_{ ext{c}}(oldsymbol{d}) = \sum_{\Omega} \|g(oldsymbol{x}+oldsymbol{u}(oldsymbol{x})) - f(oldsymbol{x})\|_2 \ & \Phi_{ ext{m}}(oldsymbol{d}) = \|oldsymbol{K}oldsymbol{u} - oldsymbol{f}\|_2 \quad ext{(Neumann)} \end{aligned}$$

The regularised problem becomes:

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Regularized Global DVC



Advantages

- Continuity of sought displacement field
- Natural regularization
- Mechanically admissible solution
- Straightforward link with simulations
- Can work for non-elastic problems

Global DVC in **Spam**

- Recently implemented
- Looking for nice data to test it!

Bridging the gap between images and FE models



Bridging the gap between images and FE models



Stamati O., Roubin E., Andò E., Malecot Y.: Tensile failure of micro-concrete: from mechanical tests to fe meso-model with the help of x-ray tomography, Meccanica (2019)

Multiple modalities



X-ray scan



Neutrons scan from D50 (NeXT, ILL)

Multiple modalities



X-ray scan

Neutrons scan from D50 (NeXT, ILL)

$$\mathcal{T}(\widetilde{\Phi}) = rac{1}{2} \sum_{\boldsymbol{x} \in \Omega} \left(f(\boldsymbol{x}) - g(\widetilde{\Phi} \cdot \boldsymbol{x}) \right)^2$$
 ?
Multimodal registration

A solution

Construct a functional $\Phi(f_x, f_n)$ based the joint histogram $p(f_x, f_n)$.



Tudisco, E., Jailin C., et al.: An extension of digital volume correlation for multimodality image registration, Measurement Science and Technology (2017)
Roubin E., Andò E., Roux S.: The colours of concrete as seen by x-rays and neutrons, Cement and Concrete Composites (2019)

Multimodal registration



MMR in Spam

- Online tutorials and examples
- Used in many published works

Going further

- Enhance spatial resolution of neutrons
- Kinematics that map one phase to the next image

General information



spam 0.7.1.0		✓ Latest version
pip install spam 🕒		
Software for the Practical Analysis of I	laterials	
Navigation	Project description	
Project description	Itemse Give pipelme passed coverage 102,00% pypi package 0.7.1,0 [055 10,2110	05/joss.02286
Release history	Snam is a niece of Puthon software huilt upon NumPu and SciPu for the analysis and	manipulation of 3D and 2D data
🛓 Download files	sets in material science, be they from x-ray tomography, random fields or any other s	ource.
	A number of common functions are provided that are either lacking or slow in Nump	y and Scipy, which are expected
Verified details	to be used by users within new python scripts. These functions are in the tools/ direct with random fields, morphological operations, digital image correlation, and labelled	tory, and include tools to work d images. Some of spam's
These details have been verified by PyPI	functions transparently call C/C++ functions for speed.	
Maintainers	Some user-callable scipts are also provided – they are more complex pieces of code to functions and which have a command-line interface. For the moment the scripts are 2	hat combine a number of 3 different image correlation
edwardando	techniques.	
P. 65	Please have a look at our online documentation for:	
(U) eroubin	Installation instructions	
gustavoPinzon	<u>General introduction</u>	
	Examples And a sumber of debiled tylesials	
O ostamati	And a number of detailed (dionals	
	If you find bugs, need help, or want to talk to the developers, we use a <u>element.io/ma</u> organisation, please join it <u>here</u> and come and talk to us – it is easy, there is a chat cli	atrix.org chat room for ent that can run in your web
	broswer. All you need to do is choose a user name!	

Stamati, Andò, Roubin: Journal of Open Source





spam 0.7.1.0	✓ Latertversion	
pip install spam 🕒	Released: Mar 6, 2024	
		downloads 290k
Software for the Practical Analysis	of Materials	downloads/month 4k
Navigation	Project description	downloads/week 647
Project description	licence (GRA3) pipetine passed coverage 1020000 pppi package 0.71.0 [055 10.21105/jiss.02286.	
Release history	Blowsbordstemmite are line chail (He)	
🛓 Download files	sets in material science, be they from x-ray tomography, random fields or any other source.	
Verified details These details have been verified by PyPI	A number of common functions are provided that are either tacking or show in Numpy and Scipy, which are expected to be used by users within new pythom scripts. There functions are in the toda/ directory, and include tools to work with nandom fields, morphological operations, digital image correlation, and labelled images. Some of spam's functions transparently; and (C-F unictions for speed.	8
Maintainers	Some user-callable scipts are also provided – they are more complex pieces of code that combine a number of functions and which have a command-line interface. For the moment the scripts are 3 different image correlation	Software, 2020 (Citatio
edwardando	techniques.	
eroubin	Please nave a look at our online documentation for: Installation instructions	
gustavoPinzon	General Introduction Examples	
ostamati	And a number of detailed tutorials	
		H'new to used
	If you find bugs, need help, or want to talk to the developers, we use a <u>element.io/matrix.org</u> chat room for organisation, please ioin it here and come and talk to us – it is easy, there is a chat client that can run in your web	Easy to use!!



pam documentation

		≡			
SPal	ntation	Introduction			
Q, Search ctr	.1 + к				
Getting started		Welcome to spam			
Introduction		Welcome to spam - The Software for the Practical Analysis of Materials.			
Installation	~	This is a Python package for handling and correlating 3D fields for applications in material science. Spam has			
Getting inspired		evolved to cover needs of data analysis from 3D x-ray tomography work and correlated random fields with mechanical applications. Seem is first and foremost a measurament package, and is divided into the following			
Gallery of Tutorials	~	toolkits:			
Gallery of Examples	~				
Scripts in sparn		DIC and deformation: Tools for measuring the transformation between 2D and 3D images,			
Getting technical		containing a non-rigid image correlation engine			
Conventions		 label; tookit to measure and manipulate labelled images, where discrete particles are labelled with interver wovel natches. 			
Tips & tricks	~	mesh : Toolkit for generating and manipulation 3D spatial meshes. In spam tetrahedral meshes are			
Indices and tables		principally used			
Repository @		kalisphera : Toolkit for generating analytical partial volume spheres, useful for testing			
Community		excursions : Toolkit for the excursion set of correlated random fields theory			
List of publications		Research Table and the balance for a few seconds of here seen has been used in a definite difference. More			
How to Contribute		Prease see <u>loos provided</u> below for a rew examples of new spam has been used in published interature. You'll find more in-depth discussion in the various Tutorials which introduce our Python function and our more			
Chat with us Ø		complex scripts, and downloadable ready-to run examples of the Python functions provided in the <u>Gallery of</u> Examples. Don't forget to browse what Python functions are available in the <u>module index</u> .			
		Please follow the Installation instructions to install spam.			
		How to cite spam			
		If you find this project useful, please cite:			

5(51), 2286, https://doi.org/10.21105/joss.02286

III Contents Welcome to spam How to cite spam Come and Chat! Tools provided

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- Installation instructions •
- Tutorials
- Examples •
- Module indices •
- Code repository •
- Communication
- How to contribute



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				Stan ⊕				
Pri	(L) Search or g			P master v span / + v		History Find file Edit - Code -	Project Information Software for Dustrial Analysis of Materials	
SI *	spam Pinned			Merge branch 'docs' into 'master' Olga Stamati aufocred 3 weeks ago				
_				Name	Last commit	Last update	1º 60 Branches	
86							S 3 Releases	
60 - 1								
10	Code Brand						© READINE © ONU OPLy3	
ø	Deploy							
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Ē.								
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				🧼 setup py	all scripts in new format and out of scri	2 months ago		

- Source code
- 93% test coverage
- Reporting issues
- Contributing!

https://gitlab.com/spam-project/spam



Valais, Switzerland 18-21/07/2023



https://www.spam-project.dev/workshops/2023/07/

Villar d'Arène, France 6-9/10/2024



https://www.spam-project.dev/workshops/2024/10/



Valais, Switzerland 18-21/07/2023



https://www.spam-project.dev/workshops/2023/07/

Villar d'Arène, France 6-9/10/2024



https://www.spam-project.dev/workshops/2024/10/

Registrations are open !

People involved



• Core-developers



People involved



• Core-developers



• Contributed with code



People involved



• Core-developers



• Contributed with code



• Contributed with ideas

