

CCPi Working Group Meeting – Monday 12th Jun. 2017

Atlas Visualisation Facility, Rutherford Appleton Laboratory

DRAFT Minutes

Attendees – in person at RAL:

- Daniil Kazantsev (DK)
- Jakob Sauer Jørgensen (JJ)
- Martin Turner (MT)
- Ron Fowler (RF)
- Srikanth Nagella (SN)
- Graham Davis (GD)
- Andrew Ramsey (AR)
- William Hallett (WH)
- Mark Basham (MB)
- Ke Deng (KD)
- Nghia Vo (NV)
- Edoardo Pasca (EP)

Attendees – Remote VC links:

- Philip Withers (PW)
- Sarah-Jane Clelland (SC)
- Kris Thielemans (KT)
- Manuchehr Soleimani (MS)

Apologies:

- Jay Wartnett
- Stefan Mairhofer
- Erica Yang
- Peter Lee
- Winfried Kockelmann
- Hamid Dehghani
- Farah Ahmed
- Bill Lionheart

Minute	Item	Action
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12.06.00	<p>The meeting began and the attendees introduced themselves. MT said that CCPi had provided various letters of support for Fellowship; Llion Evans and Marcus Hanwell in Jan 2017; for Ben Thomas (CCPETMR) and Lee Margetts (CCPi) in Jun 2017 (RSE fellowships). MT mentioned CCPi's inclusion in an EPSRC Panel to determine an equipment roadmap in Tomography. First meeting is on the 26th June. PW raised concerns that this consultation process is dragging out. Initially EPSRC were going to make the call for a Tomography Medium Scale Facility in autumn 2017. He would like to know when the committee is due to report back.</p> <p>Action – MT to get timetable from EPSRC for the MSF call.</p> <p>Update: Call is now due after the EPSRC Technology Roadmap in Tomography is released in January 2018.</p>	MT
12.06.01	<p>Agenda Item 1 – Actions from previous meeting</p> <p>MT reviewed the action list from the last meeting. In future many of these actions will transfer to SN or EY.</p> <ul style="list-style-type: none"> • <i>Visiting fellows suggestions (All). Ongoing</i> • <i>Seek e-Science journal for reconstruction work.</i> MT reported that various appropriate journals are available, including SoftwareX. MS is investigating a new journal. Closed. • <i>Arrange talks on Savu , IMAT and Avizo frameworks.</i> MT said that new developments in this area will be discussed by SN in the talk on CIL. Ongoing. • <i>Announce training courses on the CCPi email list.</i> This is now being done. Closed. • <i>Encourage people to add data sets to Zenodo.</i> New data has been added Ongoing • <i>Case studies on Beam Hardening, Quantification, SimpleFLEX.</i> These would be very useful to have Ongoing. • <i>Contact NPL to see if they can make use of Zenodo site for their data sets.</i> MT said that NPL have a meeting next month on Dimensional X-ray CT which will be announced via the CCPi email list tomorrow. Closed. • <i>For high speed files transfers to/from DLS ask local admins to allow firewall bypass.</i> MT said that DLS to UoM rates of 1TByte/hour had been achieved which was sufficient for current requirements. Closed. • <i>GD and BL to discuss editing new Phil Trans issue on reconstruction.</i> Hope to get a list of authors soon. Ongoing. • <i>Suggest articles for new Phil Trans issue.</i> Ideas for further issues included: Rich tomography, pre-processing for CT. Ongoing. • <i>Arrange visit by Astra developers.</i> MB had talked to Astra people and expected to arrange a visit after the summer. • <i>Updated proposal for joint CCPi/CCP PET/MR workshop late next year.</i> MT said that BL and others had been exchanging emails and a joint workshop on Bayesian reconstruction was being considered which could benefit both flagship proposals. Ongoing. 	<p>All</p> <p>SN</p> <p>EY/SN/RF</p> <p>SN</p> <p>GD/BL</p> <p>All</p> <p>MB</p> <p>BL/KT</p>

	<ul style="list-style-type: none"> • <i>Discuss policy on CCPi support for attending training courses.</i> MT said that there had not being any demand for this and if it did arise it would be considered on a case-by-case basis. Closed. 	
12.06.02	<p>Agenda Item 2 - CCPi related activities for last 6 months and future reporting</p> <ul style="list-style-type: none"> • The reporting of CCPi activities to EPSRC is changing. SN said that in future reports need to be more descriptive so that non-experts can understand the contributions made by CCPi activities. The previous style had been to give short "bullet point" summaries of the main achievements with limited detail. • MT reported that a new developer (EP) had joined STFC and is now working on both CCPi and CCP-PET/MR projects. • With the formal release of the Core-Imaging-Library (CIL) due at the end of this month there is a need to identify new codes which could be added to it. One possibility was the DVC code from Brian Bay. Other suggestions are welcome. Action: SN to check if Brian Bay's code could be added to CIL. Action: All - Suggestions for other codes to include in CIL. • Exchanges: MT reported: <ul style="list-style-type: none"> ○ Sponsoring X-ray fringe meeting, following on after working group. ○ Three European visitors: Andy King, Asa Barber and Margie Olbinado. ○ BL hosted CCPi meeting with Soren Schmidt, Markus Strobl, Morten Sales ○ A lab based exchange involving Russell Garwood/Imran Rahman for Manchester Museum artefacts for ISIS/IMAT neutron tomography. • Seminars: MT listed the seminars CCPi has arranged and presented at over the last 6 months, including talks on SuRVoS (DLS) and Contour Tree (Simple Flex) segmentation. The latter is included in CIL. • Exhibitions: CCPi was presented at three exhibitions, Supercomputing November 2016, Manchester Regus Professor in Materials Event April 2017 and British Science Week March 2017. • MT listed the training events CCPi had been involved in. These include Avizo training, using CCPi NeXuS reader, SuRVoS workshop and "3D and 4D imaging: Automation of data analysis". • Standards: MT had attended and reported on two meetings of the BSI XCT panel in January and March. The emerging first standard will be a single phase material (metal/air) where beam hardening is seen as a limiting factor. The next meeting is the dimensional X-ray CT conference in Warwick (13th July 2017). • Developer's days for Flagship and CIL: Two events were held: <ul style="list-style-type: none"> ○ Pre-workshop meeting, 20 March 2017 ○ Phone conference update, 11 May 2017 • Papers/videos: <ul style="list-style-type: none"> ○ Total of 8299 views on CCPi channel ○ 19 touch screen example data sets 	<p>SN All</p>

	<ul style="list-style-type: none"> ○ New data sets on zenodo including new links from Llion Evans. Data sets of up to 50 GBytes are possible on zenodo. ● CCPi supported events: <ul style="list-style-type: none"> ○ Advances in X-ray Imaging workshop (RAL/RCaH) 13 June 2017 ○ Dimensional X-ray Computed Tomography Conference, 13 July 2017 at Warwick ○ ToScA Conference 6-8 Sept 2017, Portsmouth. <p>MT reported that ToScA USA conference occurred on the 6-8th June 2017. PW asked about attendance numbers. Action: MT to find numbers.</p>	MT
12.06.03	<p>Agenda Item 2 - Flagship Update</p> <ul style="list-style-type: none"> ● DK gave an update on the CCPi Flagship work. He discussed the work on reconstruction of Multichannel CT and the RT-MCT toolkit that is being developed to do this. Both DLS and ISIS are able to generate multichannel tomographic data. DLS will help integrate the toolkit into Savu. The project is described on the CCPi website. More details of the project will be given in the afternoon session. 	
12.06.04	<p>Agenda Item 3 – Software developments</p> <ul style="list-style-type: none"> ● SN gave an overview of CCPi software developments over the past 6 months. <ul style="list-style-type: none"> ○ A paper on the beam hardening software is to be submitted to the Journal SoftwareX. ○ Work has focused on the upcoming release of the new core imaging library (CIL). ○ The first release of CIL will use an Anaconda channel for easy installation of the Python bindings to the algorithms. 	
12.06.05	<p>Agenda Item 5 – Drishti-Prayog user guide</p> <ul style="list-style-type: none"> ● MT described the Dristi-Prayog user guide which is now available via the CCPi website. This is an updated version of the DLS guide and allows fast conversion of data into a format for display on touch screen devices. This is useful for displays at meetings with a touch screen panel connected to a laptop. MB asked if a workshop session could be arranged on getting data into Drishti-Prayog. SN agreed that this would be useful. Action: SN to investigate. 	SN
12.06.06	<p>Agenda Item 6 – IMAT experiment with ICAL/Oxford/Birmingham</p> <ul style="list-style-type: none"> ● SN gave details of an experiment that was performed in the IMAT commissioning phase to image a fossil – that of a crab. Some initial reconstruction results were reported. Current images were obtained with “white beam” at 2000x2000 resolution and 1400 projections. In future time of flight data will allow multichannel imaging. MT said that there may be potential for others to get time on IMAT in the commission phase. 	
12.06.07	<p>Agenda item 7 – New actions and milestones</p> <ul style="list-style-type: none"> ● The milestones for 2016-17 were reviewed and new ones for 2017-18 discussed. SN said that various milestones had been identified for the upcoming release of the CIL software. PW said that it is important to have named lead individuals for each key task. 	

	Action: Assign names to tasks (SN/EY).	SN/EY
12.06.08	<p>Agenda Item 8 – Web site items</p> <ul style="list-style-type: none"> • SN gave a brief overview of web site updates. The site is based on a Drupal content management system. Recent additions include the web page for the CCPi flagship project. 	
12.06.09	<p>Agenda Item 9 – Update from CCP PET-MR</p> <ul style="list-style-type: none"> • KT gave an update on work within the sister CCP. <ul style="list-style-type: none"> ○ The first public release of version 0.9 of the SIRF software is due tomorrow. It provides MATLAB and Python interfaces to the MR and PET reconstruction packages along with simulated data sets. ○ The PET-MR flagship proposal was approved and will start from the end of September for 3 years. ○ The proposed joint workshop with CCPi on Bayesian methods is a good idea. A date still needs to be set. MT suggested contact by email to set a meeting for September or October. Action for this set previously. 	
12.06.10	<p>Agenda Item 10 – Short talks</p> <p>Image processing for tomography – Nghia Vo</p> <ul style="list-style-type: none"> • NV described algorithms used by DLS for image pre-processing. These address various problems such automatic correction for centre of rotation errors, distortion correction, ring artefacts and alignment issues. The correction algorithms will be included in SAVU. • PW commented that similar problems were seen by people on beamline I13 and he offered to put NV in contact with them. Action: PW to provide contact information to NV. • Other work included Image reconstruction, covering helical, time series, high speed and limited angle scans. For the limited angle data good results were seen with 30 degrees missing data. <p>Core Imaging Library (CIL) – Sri Nagella</p> <ul style="list-style-type: none"> • SN gave an overview of the new Core Imaging Library which will be used to package algorithms of use to the community with a common interface. • The documentation will make use of “read-the-docs” format for easy access and updating. • The aim is to have regular release cycles, with two updates per year. • The first release is expected by the end of June with Python bindings (first regular v-conf 21 June 2017, 11am). • Next release to focus on Avizo, ImageJ and Savu interfaces; and missing wedge. • MT said that named people should be responsible for each component of the release and should aim to do comparisons e.g. between CGLS in CIL and the Astra versions. • PW suggested checking if Brian Bay’s Digital Volume Correlation code could be included in CIL. Action set previously. • SN described the segmentation possible using the SimpleFLEX 	PW

	PET/MR workshop late next year		
12.06.02	Request additional codes to include in CCPi quantification software	All	
	Contact Brian Bay to see if DVC code can be included CCPi quantification software (CIL)	SN	
	MT to find ToScA USA attendance numbers for PW.	MT	
12.06.05	Arrange workshop session on getting data into Drishti-Prayog	SN	
12.06.07	Assign name to tasks for CCPi actions and milestones.	SN/EY	
12.06.10	PW to provide contact information to NV for users on I13 with image processing issues.	PW	
12.06.11	Submit ParaView paper to EGUK	MT	
12.06.13	Monitor upcoming workshops/events.	MT	

Appendix A: CCPi Hosted 2nd X-Ray Fringe Meeting - 12 June 2017, 14:00-17:30 in Atlas Visualisation Facility at RAL

The Fringe Meeting was a pre-meeting to the (13 June 2017) "Advances in X-ray Imaging" Workshop, held in DLS, RAL with CCPi / RCaH Sponsorship. Their speaker program is at <https://advances-in-x-ray-imaging-ii.eventbrite.co.uk> and had a full sell-out attendance of ~70.

The Fringe meeting creates a forum space for people to think a bit outside the box and be less conventional in ideas than at the workshop. Attendance numbers (26 people from 13 different institutions):

- Martin Turner martin.turner@manchester.ac.uk
- Daniil Kazantsev daniil.kazantsev@manchester.ac.uk
- Nishtha Chopra nishtha50376@gmail.com (Queen Mary, University of London)
- Jakob Jorgensen jakj@dtu.dk (Manchester now)
- David Eastwood david.eastwood@manchester.ac.uk
- James Carr james.carr@manchester.ac.uk
- Zepeng Lv lv.zepeng@manchester.ac.uk
- Siyuan Chen siyuan.chen-5@postgrad.manchester.ac.uk
- Tim Burnett timothy.burnett@manchester.ac.uk
- James Whiston j.whiston@warwick.ac.uk
- Anna Martinez anna.martinez@hsl.gsi.gov.uk
- Jiawei Mi j.mi@hull.ac.uk
- Nghia Vo nghia.vo@diamond.ac.uk
- Ke Deng dksjtu@gmail.com
- Daren Batey darren.batey@diamond.ac.uk
- Andy King king@synchrotron-soleil.fr
- Asa Barber asa.barber@port.ac.uk
- Margie Olbinado margie.olbinado@esrf.fr
- Kate Dodson katherine.dobson@durham.ac.uk
- Sam Cooper samuel.cooper@imperial.ac.uk

Organisers and local coordinators at RAL:

- Loic Courtois loic.courtois@3dmagination.eu
- Kamel Madi kamel.madi@3dmagination.eu
- Joe Kelleher joe.kelleher@stfc.ac.uk
- Jenny Woods jenny.woods@manchester.ac.uk
- Sri Nagella srikanth.nagella@stfc.ac.uk
- Ron Fowler ronald.fowler@stfc.ac.uk
- Edoardo Pasca edoardo.pasca@stfc.ac.uk , Erica Yang erica.yang@stfc.ac.uk (apologies)



Fringe Agenda Points:

Two key topic items were discussed on the design of future facilities:

The Future of XCT - 'unusual' coding solutions across the CT pipeline. Two main presentations were given to consider ideas;

1. New CCPi Flagship grant for 'unusual and upcoming' Multi Channel CT reconstruction and missing wedge/ poor data reconstruction (DK/JJ) considered the initial data capture process then processing stages required to create the 'best' 3D volumes, and;
2. Sam Cooper, described TauFactor a tomography tool to calculate tortuosity factor, volume fractions, etc. as a potential post-processing stage for the 3D volumes using HPC data analytics. The software is a Matlab plugin provided under an open source license.

There were questions and comments;

- What other joint reconstruction methods could benefit from this Multichannel CT reconstruction process: - even possibly considering usual colour RGB imaging as opposed in greyscale (i.e. 2D instead of 3D).
- Links with PET-MR for example and other medical experience, which combines modalities, and the use of HyperStacks (a specific definition in certain code bases).
- Discussion on current image size for multi-channel CT – this could be 400x400x400 by 200 channels [so every voxel in a 400³ dataset is a spectrum of 200 values]. This size it was commented on would be computable using current HPC (GPU clusters).
- What is the similarity with phase reconstruction that considers a distance function (as a 4D function – but only has a few extra reconstructions required). Good discussion on which materials are appropriate that could be differentiated from one to the other method.

The EPSRC XCT Roadmap outline and discussion was described from the website by MT with cross-links to the new BSI standards for XCT (currently in progress XCT panel - TDW/4/4/1). Open discussion on various topics and needs for the community to create a series of “mountains” rather than a single “Everest” that need to be climbed; this would be a metaphor for a new XCT Roadmap vision.

A series of short feedback points came from invited speakers Darren Batey, Beamline I13, Diamond Light Source 'Ptychography: Looking beyond the lens'; Tim Burnett, Henry Moseley X-ray Imaging Facility, 'Multiscale 3D microstructure analysis with site specific targeting through correlation of X-ray CT and FIB-SEM serial sectioning', Andy King, Soleil 'Combining tomography and diffraction ' and Margie Olbinado, ID19, ESRF 'Million frames per second hard X-ray phase contrast imaging using synchrotron.

There were questions and comments and good ideas, including;

- **Multi-scale is essential** and is both a local strength at certain locations, but would improve by sharing – collocating facilities together. This is also considered as an important industrial ‘research’ service to be offered. An example was given for “following a crack” from the large source to the very high resolution tip that would require multiple XCT machines.
- **Other mixed facilities** were considered enabling new understanding of materials; including XCT with microscope (SEM) that would be correlated. Or integrated XCT with 3D additive manufacturing facilities (including neutron and/or gamma ray tomography).
- Special sample holders need to be sharable – **specialist rigs** can be expensive and should be available and cross-purpose between the lab and the national facilities. Creating some universal standard would allow samples to be easily scanned in different locations (also has standard checking as an additional feature).
- Industrial users commented on the need for a **‘complete dataflow’ system** to be available; that would enable bespoke practices. So this may allow multiple capture techniques to even larger multiple data analytics code to be applied to many (1000’s) of samples and techniques.
 - The **term ‘industrial ambition’** was considered critical.
- There is **a need for a well-funded network** to be present (setup – an enhanced CCPi offering) to provide multiple features including; offer seed funding to create early stage outcomes before larger EPSRC project proposals would be submitted; better cross facility exchange scheme; and better exchange of national/international expertise and practice.
 - Comment that this network could **‘look sideways’ at non-EPSRC users**; including other research councils, biological, rock, etc. that would be a future route for the combined RC network.
- In Materials Science, a focus was to consider the range of **very new materials** that are being considered and discovered – perhaps new imaging (robotic and mass-analysis methods) to be discovered from **Machine Learning / Deep Learning** from data archives.
- Role in **education** was also considered essential; to create CDT and other courses including specialist training areas. This was repeatedly considered an important “mountain” to climb as there are not enough PhD / postdocs and then undergrads ready in the UK. So included basic undergraduate courses in ‘3D and tomography’ – and not just in Maths and Engineering.
 - Discussion covered the range of courses that should be available; week long detailed physics based tomography course, to a set of short introduction to tomography courses, some focussed on ‘what people need to know’ so ...sample preparation; rigs; mounting techniques; scanning setup; processing....
 - Explicitly have training from lab to synchrotron use.
- Another “mountain” to climb would be to use the network to improve the **disconnect between lab based and national based** – synchrotron and neutron - facilities. Need to define currently “What cannot be done at the laboratory but can be done in mid-range or national facilities”

- Scale, Speed, 4D (even 5D) and other specialisms were also considered a future problem; especially in the national facilities but in mid-range ones as well - including very large length and time scales and creating very large datasets (very relevant to both research and industry)

My early text and opening thoughts (by MT):

Reminder that the CCPi (tomographic Imaging) network has a growing user list of 350 people – and other community XCT lists exist, each in their hundred's; NPL's and ToScA. From the principles of a Roadmap for the EPSRC that;

- "supporting suitable and well rationalised technique-based roadmaps e.g. NMR spectroscopy..."
- "current UK capital infrastructure ... which in turn may lead to more and/or better equipment sharing"
- "... will have community buy-in; demonstrated through applicants taking it into consideration"

Initial proposal ideas list numerous technologies issues; including but not limited to increasing scale quantification; (multi-scale) imaging analysis and derived; chemistry, biology, engineering values - stress, etc. and integration with alternative processes.

I see two main outcomes in the UK;

1. simpler imaging systems - similar to the development of SEM where cheaper lab based facilities with a kite-mark of standardisation are affordable to all groups (£<50K), and installed with NPL Guides of Practice to 100's of groups within the UK from small university research labs to SME manufacturing facilities; and
2. high-end very fast and multi-channel/energy imaging systems - creating large data deluge that allow multiple parameters to be recorded at once and continually giving physics, biology, chemistry and engineering values for sub/global-parts of an object under multitude types of influence (different environment in-situ rigs); changing temperature, pressure, shearing, catalytic reaction etc.

So many places will have one or a few systems and some will have a multitude of systems – over many scales/ (in-situ)rigs / and all being 4D or 5D (temporal etc) and thus also becoming big data problems; and all linking to national specialist one-off systems when needed.

Appendix B: VR Aside for Fun - 12 June 2017, 12:00-14:00 in Atlas Visualisation Facility at RAL

Over lunch we setup the Virtual Reality example from Unity code that allows 3D volume visualisation to be incorporated within a head mounted setup (HTC Vive). This used the CCPi publically available tomographic 'mobile phone data set' to demonstrate real data to this community.



Appendix C CCPi Milestones and targets

Targets for the mid-term review:

Networking Targets

User base:

- 300 members of network
- Expand to include neutron tomography

International links

- 3 International Fellows visits

Links with industry

- 5 companies attend our annual conference/year
- 5 Industrialists attend training courses/workshops

Feedback from workshops/training

- 100 different people have attended workshops/training

Outreach

- 2 how-to videos/webinars
- 5 outreach videos for schools available on youtube
- 5 touch-screen 3D models

Software Development Targets

New scientific functionality added

- Beta version of our image acquisition and analysis workflow capable of running our tools running on synchrotron data
- 3 pre-processing analysis routines added
- 4 post-processing analysis routines added
- 2 reconstruction tools added for multi-modality

Ability to run on new platforms

- 2 GPU/Phi/FPGA version of codes piloted

New algorithms / Increased efficiency of code

- Beyond 3D – multimodal reconstruction
- Fewer projection methods
- Fully documented iterative algorithm for cluster systems

Papers

- 8

Complementary Funding Targets

- 2 parallel funded projects (industry or Research Council)

Coding Milestones are related to above and are more relevant to STFC targets inside work plans. The current list is at <http://tyne.dl.ac.uk/twiki/bin/view/Visualisation/CCPiTomo> .