CCP-SAS: New developments in computational modelling of X-ray and neutron scattering curves

Virtual Satellite Meeting at the 60th British Biophysical Society Meeting, UK

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NIST and UCL

CCP-SAS
A Joint EPSRC-NSF Software Project

CCP-SAS

Usual Zoom rules apply:

Please keep mikes off.
Please post questions in the chat throughout the talks.
The chair will read them to the speaker at the end.
Auto-captions are available to those wishing to have them.

(1) What is CCP-SAS?
(2) Applications?
(3) Achievements?
(4) Developments/Future

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Scattering problem

Scattering is directly related to the organization of atoms within a material and thus a powerful tool for the elucidation of the detailed microstructure of materials.

BUT

Maximizing the information extracted from the analysis requires:

1) Using all a priori information available to constrain the solution.
2) Careful posing of the question and design of experiment
3) Can become computationally challenging

Is used by a wide variety of scientists from geology to biology, from physics to chemistry etc. – Not all experimentalists in these fields have the skills to extract the most information from the data

MEANING: The modelling dilemma – to model - or not to model.

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CCP-SAS in a nutshell

Create new and enable existing computational tools to model scattering data in real space using modern MD and MC methods as well as applying constraints from other experimental techniques
AND
dramatically improve their accessibility by non-experts.

MEANING: Interpret SAS curves at a molecular or atomistic level, not as solid objects or envelopes

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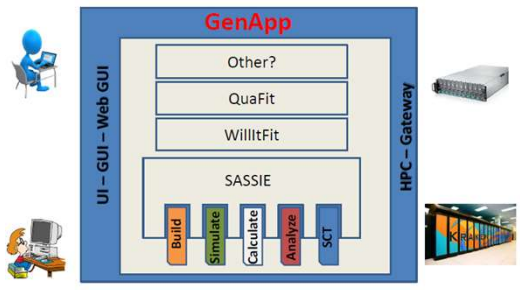
The CCP-SAS Solution



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Good vs. successful software

The most brilliant software in the world .....

If nobody ever uses it

Or it fails to be maintained long term (after the honeymoon is over)

IS A COMPLETE AND UTTER FAILURE

MEANING: The need to build a community around CCP-SAS and promote this.

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(1) What is CCP-SAS?
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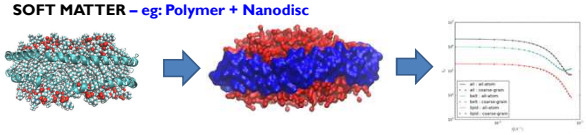
Session 1 this afternoon will look at applications

Applications are broad ranging

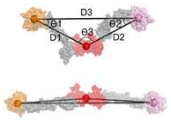
SOFT MATTER – eg: Polymer + Nanodisc



BIOLOGY AND BIOTECHNOLOGY

eg: Antibody + Glycans

G K Hui *et al.*, Biochem. J. (2015), DOI: 10.1042/BJ201506



eg: Complement

R. Nan *et al.*, Strructure. (2017), DOI 10.1016/j.str.2016.12.014

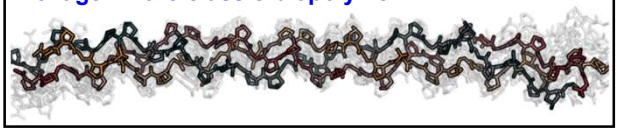
eg: Hfq + RNA

Y Peng *et al.*, *PNAS* (2014), DOI: 10.1073/pnas.14101 14111

Outcomes give molecular structures that clarify biological function

IgG1 antibodies – widespread utilities

Collagen – the classic biopolymer



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Usage of SASSIE-web on the HPC at Tennessee, USA

May 2016 – 273 registered users
Sep 2020 – 952 registered users

Period	Hours CPU per year	Active users	Power users >100 jobs
Beta period Jun15-May16	8500		
Jul17-Aug18	24900	134	18
Jul18-Aug19	35000	158	24
Jul19-Aug20	44900	104	12

CCP-SAS publications in good journals

Year	All	Biology	Techniques	Soft Matter	Biopolymer
2020	4				
2019	12				
2018	5				
2017	8				
2016	14				
2015	9				
2014	10				
2013	7				
Totals	69	39	5	18	7

Biology – includes PNAS, Structure, JBC – a good spread of the stronger journals

Talks and tutorials worldwide

ILL and ESRF, May 2015

Argonne National Laboratory, USA, Sep 2016.

Cosener's House, ISIS and Diamond Light Source, Jan 2017.

INSER, Mohali (Delhi), India, Sep 2017

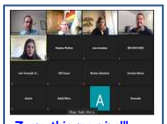
IIS, Bangalore, India, Sep 2017

NIBGE, Faisalabad, Pakistan, May 2018

ILL, SimSAS Meeting, Apr 2019

ISIS neutron training course, Jun 2019

24th International AUC Workshop, Christchurch, New Zealand, Aug 2019



Zoom this morning!!!

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(1) What is CCP-SAS?
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Session 2 this afternoon will look at the future – where are we on the computing side?

Conclusion – CCP-SAS is on the way to becoming established for the atomistic modelling of macromolecules by scattering