

CCP-SAS

a

Collaborative Computational Project for Small Angle Scattering

goals, achievements and aspirations

4th Annual CCP-SAS Project Workshop

June 19, 2017



Engineering and Physical Sciences
Research Council



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- 2) Careful posing of the question and design of experiment
- 3) Can become computationally challenging

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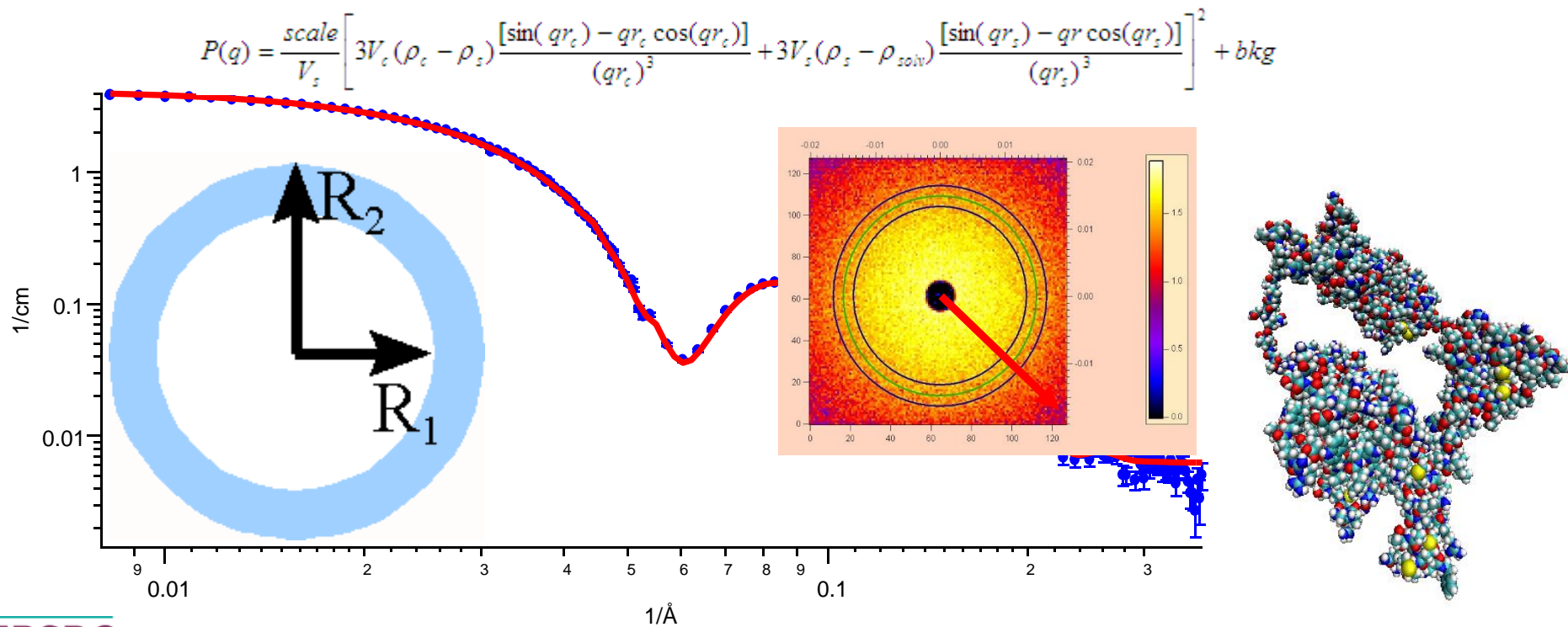
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Is used by a wide variety of scientists from geology to biology, from physics to chemistry etc. – Not all experimentalists in these fields have the skills to extract the most information from the data

SAS Analysis: approach I

Either postulate idealized geometric shape and parametrize its scattering, or when systems that have little symmetry and where the possible variations could not be captured by a single analytical model, generate candidate structure in real space and FFT to compare to data – iterate.



SAS Analysis: The Next Level

- Apply modern MD and MC simulation methods to generate ensembles of possible structures coupled with high throughput computing methods to screen for reasonable structures that match the data and gain molecular level insights
- Use as much a priori information as possible from other techniques such as AUC, NMR, EM etc
- And make it accessible to the bench scientist

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.

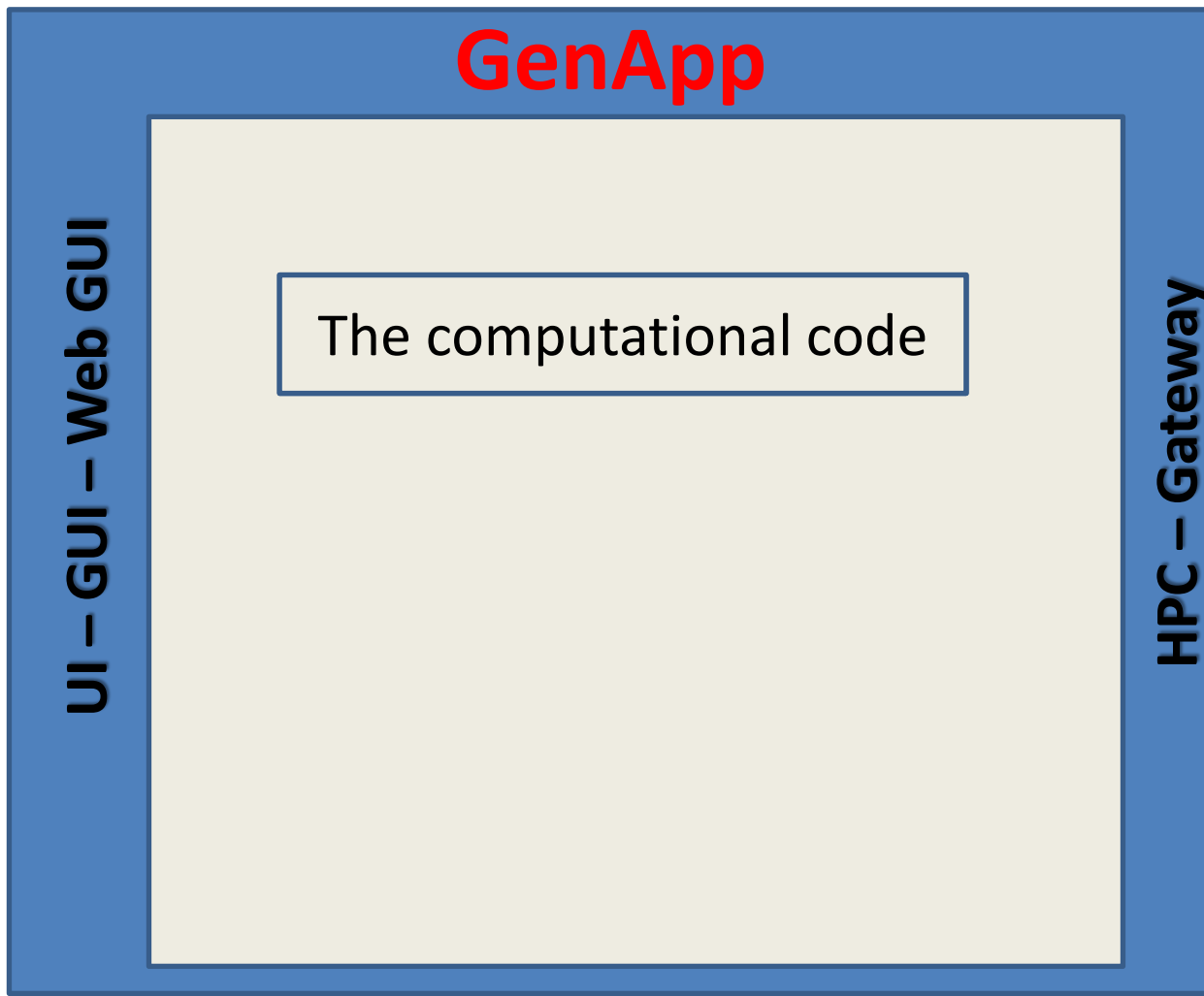
The CCP-SAS Solution



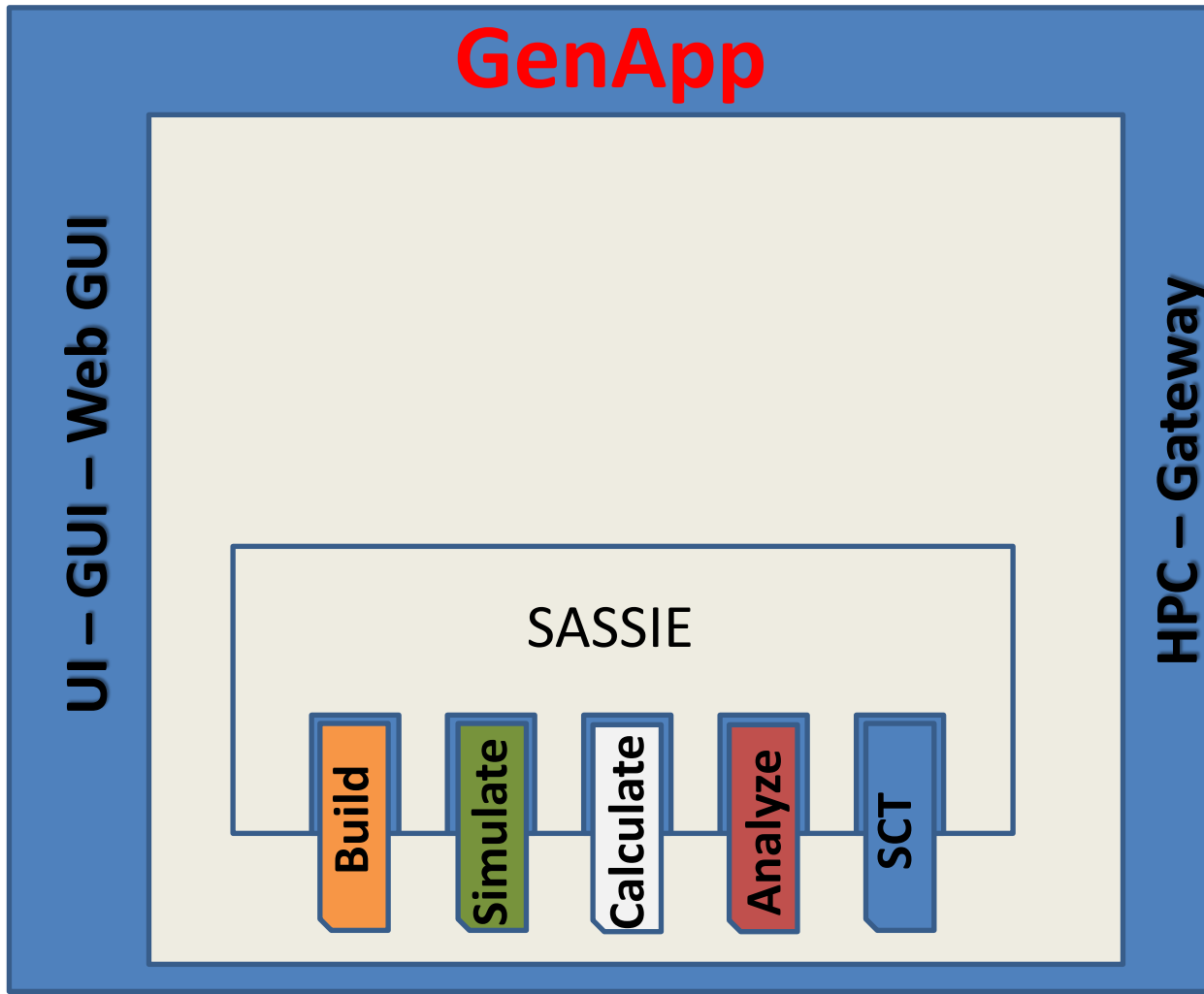
The computational code



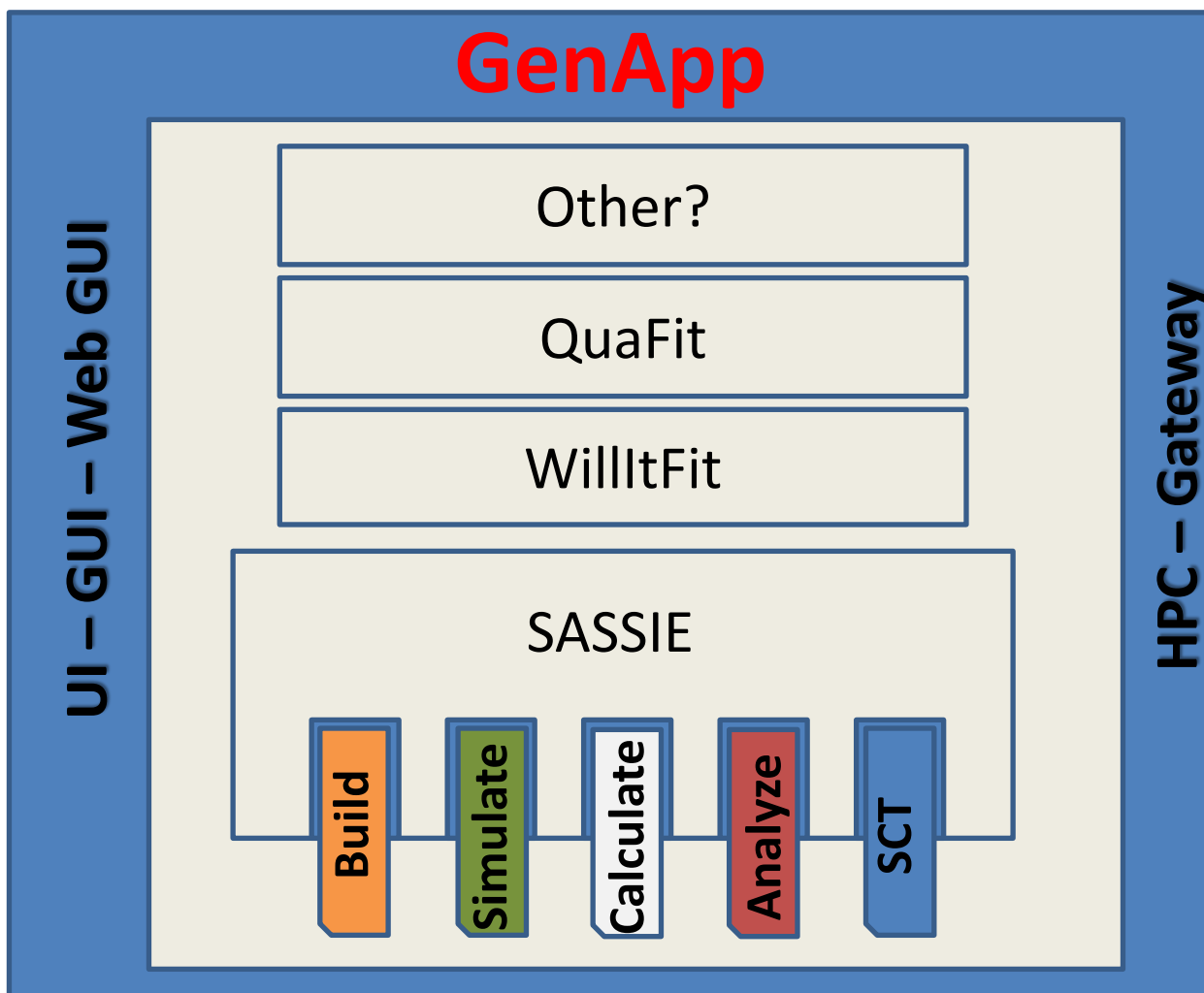
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Good vs. successful software

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

How do we best resource the next stages?

- Deployment and maintenance (including training)
- Development (needs are always “infinite”)
 - More general (and or specialized) builders
 - General and robust handling of polydispersity and interactions
 - Force field development? (MGI?)
 - Proper handling of co-refinement of data from several techniques and integrated with MD?
 - Other....

And now the rubber hits the road

We will hear about many projects and ideas this afternoon and on posters while others were unable to attend.

Suggest that all benefit from a more
Collaborative (Computational) approach

We look forward to tomorrow's discussions
and outcomes!