

## Speakers

The following speakers will be present at the school:

P. Adams	<a href="#"><u>Phenix</u></a>	Lawrence Berkeley Laboratory, California, USA
D. Borek	<a href="#"><u>HKL2000/HKL3000</u></a>	Southwestern Medical Center, Dallas, USA
K. Cowtan	<a href="#"><u>Parrot, Buccaneer</u></a>	York Structural Biology Laboratory, York University, UK
Z. Dauter	<a href="#"><u>Data collection strategies, Twinning</u></a>	Argonne National Laboratory, Chicago, USA
K. Diederichs	<a href="#"><u>XDS</u></a>	Universitat Konstanz, Germany
T. Gruene	<a href="#"><u>Shelx</u></a>	Georg-August-Universitat, Gottingen, Germany
R. Keegan	<a href="#"><u>MrBUMP, CCP4 Group</u></a>	STFC Daresbury Laboratory, UK
E. Krissinel	<a href="#"><u>PISA</u></a>	European Bioinformatics Institute, Cambridge, UK
G. Langer	<a href="#"><u>ARP/wARP</u></a>	European Molecular Biology Laboratory, Hamburg, Germany
A. Leslie	<a href="#"><u>Mosflm, iMosflm</u></a>	MRC-LMB, Cambridge, UK
B. Lohkamp	<a href="#"><u>Coot</u></a>	YSBL, York University, UK & Karolinska Institute, Sweden
E. Merritt	<a href="#"><u>TLS Refinement</u></a>	University of Washington, USA
G. Murshudov	<a href="#"><u>Refmac, BALBES</u></a>	York Structural Biology Laboratory, York University, UK
R. Pannu	<a href="#"><u>Crank, BP3</u></a>	Leiden Institute of Chemistry, The Netherlands
R. Read	<a href="#"><u>Phaser</u></a>	Cambridge Institute for Medical Research, University of Cambridge, UK
T. Terwilliger	<a href="#"><u>Phenix</u></a>	Los Alamos National Laboratory, USA

# Program

## Basic Daily Schedule

<b>Morning</b>	Breakfast Lectures on theoretical background of software package(s)
<b>Afternoon</b>	Lunch Tutorials on software package(s) discussed in the morning
<b>Evening</b>	Dinner Problem solving sessions

### Exceptions:

**June 24th** is a half day and is for user safety training, beamline orientation and lectures on data collection and processing strategies. **June 25th** is for data collection and real-time processing. **June 26th** is a half day for data processing. After **June 26th** students will have access to all tutorials and tutors will be available to answer questions. Students are encouraged to use provided tutorial data as well as try their own data.

In the morning of **June 26th** lecturers and tutors will make sure software is set up right on computers, presentations are properly copied where they need to be, slides are properly displayed, etc. etc.

**June 24th and 25th**, pick up your workshop badge and binder outside of room E1100 after breakfast.

**June 26th** pick up workshop badge and a binder outside of room E1100 after breakfast.

**June 29th** is a half day. No sessions after lunch. Trip to Chicago.

## Detailed Program

Below is the detailed program for the workshop. Please check back for updates. There may be minor updates to the program before the workshop takes place but there will be no major departures from this plan.

24 June 2009			
<i>Beamline orientation and data collection training</i>		<i>Instructor</i>	<i>Location</i>
All day	<i>Registration throughout the day</i>	Sheila Trznadel	
11:30	Welcome and Introduction	B. Fischetti N. Sanishvili	A1100
12:00	<i>Working lunch</i> - Brief description of problems and crystal	Students with crystals	A1100
1:00	Data collection software	GM/CA Staff	A1100
3:30	<i>Coffee</i>		A1100
4:00	Beamline Tour	GM/CA Staff	Sector 23
5:00	All about data(data collection theory)	Z. Dauter	A1100
6:00	<i>Dinner</i>		APS Gallery
7:30	Beamline training (Hutches and goniometry)	GM/CA staff	Sector 23
8:30	Final sample preparation, scheduling of data collection, spreadsheets and sample loading	GM/CA staff	Sector 23
25 June 2009			
<i>Data collection and processing</i>		<i>Instructor</i>	<i>Location</i>
8:30	<i>Breakfast</i>		APS Gallery
9:30	Data collection and real-time processing	GM/CA staff D. Borek K. Diederichs A. Leslie	APS, Sector 23
12:30	<i>Lunch</i>		APS Gallery
1:30	Data collection and real-time processing	GM/CA staff D. Borek K. Diederichs A. Leslie	APS, Sector 23
4:30	<i>Coffee</i>		APS Gallery
5:00	Data collection and real-time processing	GM/CA staff D. Borek K. Diederichs A. Leslie	APS, Sector 23

6:00	<i>Dinner</i>		APS Gallery or Sector 23
7:30	Data collection and real-time processing	GM/CA staff D. Borek K. Diederichs A. Leslie	APS, Sector 23
<b>26 June 2009</b>			
<i>Data Processing</i>		<i>Instructor</i>	<i>Location</i>
8:30	<i>Breakfast</i>		APS Gallery
9:00	Registration	Sheila	Outside Room 1100
12:00	Welcome	B. Fischetti	Room E1100/E1200
12:10	Introduction	N. Sanishvili	
12:30	<i>Lunch</i>		APS Gallery
1:30	Data Processing using MOSFLM and Scala	A. Leslie	Room E1100/E1200
2:15	HKL2000	D. Borek	Room E1100/E1200
3:00	XDS	K. Diederichs	Room E1100/E1200
3:45	<i>Coffee</i>		APS Gallery
4:00	Twinning and other crystal growth pathologies	Z. Dauter	Room E1100/E1200
4:45	Tutorial: Data integration and reduction problem solving	All	Room E1100
6:00	<i>Dinner</i>		APS Gallery
7:00-10:00	Tutorial: Data integration and reduction problem solving	All	Room E1100
<b>27 June 2009</b>			
<i>Experimental Phasing</i>		<i>Instructor</i>	<i>Location</i>
8:30	<i>Breakfast</i>		APS Gallery
9:00	Shelxd/Shelxe	T. Gruene	Room E1100/E1200
9:45	Phaser	R. Read	Room E1100/E1200
10:30	<i>Coffee</i>		APS Gallery
11:00	Crank/BP3	R. Pannu	Room E1100/E1200
11:45	Pirate and around	K. Cowtan	Room E1100/E1200
12:30	<i>Lunch</i>		APS Gallery
1:30	Coot: An introduction	B. Lohkamp	Room E1100/E1200
2:15	Tutorial: All tutorials and problem solving	All	Room E1100

3:30	<i>Coffee</i>		APS Gallery
4:00	Tutorials and problem solving continued	All	Room E1100
6:00	<i>Dinner</i>		APS Gallery
7:00-10:00	Problem solving for volunteers	All	Room E1100

### 28 June 2009

<i>Automation Pipelines and Molecular Replacement</i>		<i>Instructor</i>	<i>Location</i>
8:30	<i>Breakfast</i>		APS Gallery
9:00	Automation in Phenix	T. Terwilliger	Room E1100/E1200
9:45	Buccaneer	K. Cowtan	Room E1100/E1200
10:30	<i>Coffee</i>		APS Gallery
11:00	MrBUMP	R. Keegan	Room E1100/E1200
11:45	BALBES	G. Murshudov	Room E1100/E1200
12:30	<i>Lunch</i>		APS Gallery
1:30	Tutorial: All tutorials Problem Solving	All	Room E1100
3:30	<i>Coffee</i>		APS Gallery
4:00	Tutorials and Problem solving continued	All	Room E1100
6:00	<i>Dinner</i>		APS Gallery
7:00-10:00	Problem solving for volunteers	All	Room E1100

### 29 June 2009

<i>Morning all tutorials and problem solving Afternoon and evening free time</i>		<i>Instructor</i>	<i>Location</i>
8:30	<i>Breakfast</i>		APS Gallery
9:00	Data peculiarities: Twinning, Pseudosymmetry	Z. Dauter G. Murshudov	Room E1100/E1200
10:30	<i>Coffee</i>		APS Gallery
11:00	Tutorials and Problem solving continued	All	Room E1100
12:30	<i>Lunch</i>		APS Gallery
1:30	Bus leaves for Chicago		Chicago
3:00	Be a tourist in Chicago		Details later
9:30	Bus leaves Chicago for Guest House		Chicago

**30 June 2009**

<b>Refinement and autobuilding</b>			<b>Instructor</b>	<b>Location</b>
8:30	<i>Breakfast</i>			APS Gallery
9:00	Refinement in Phenix		P. Adams	Room E1100/E1200
9:45	Refmac		G. Murshudov	Room E1100/E1200
10:30	<i>Coffee</i>			APS Gallery
11:00	Arp/Warp		G. Langer	Room E1100/E1200
11:45	TLS and all that		E. Merritt	Room E1100/E1200
12:30	<i>Lunch</i>			APS Gallery
1:30	Tutorial: All tutorials Problem Solving		All	Room E1100
3:30	<i>Coffee</i>			APS Gallery
4:00	Tutorials and Problem solving continued		All	Room E1100
6:00	<i>Dinner</i>			APS Gallery
7:00- 10:00	Problem solving for volunteers		All	Room E1100

**1 July 2009**

<b>Model building and validation</b>			<b>Instructor</b>	<b>Location</b>
8:30	<i>Breakfast</i>			APS Gallery
9:00	Ligands and ligand dictionary		GM and PA	Room E1100/E1200
9:40	Automatic ligand fitting with ARPwARP		G. Langer	Room E1100/E1200
10:00	PISA		E. Krissinel	Room E1100/E1200
10:45	<i>Coffee</i>			APS Gallery
11:15	Coot		B. Lohkamp	Room E1100/E1200
12:00	Tutorials and Problem solving continued		All	Room E1100
12:30	<i>Lunch</i>			APS Gallery
1:30	Tutorial: All tutorials Problem Solving		All	Room E1100
3:30	<i>Coffee</i>			APS Gallery
4:00	Tutorials and Problem solving continued		All	Room E1100
6:00	<i>Dinner</i>			APS Gallery

**2 July 2009**

<b>Finalise</b>			<b>Instructor</b>	<b>Location</b>
<b>2 July 2009</b>	<b>Problem Solving</b>			<b>Location</b>
9:00	Tutorials and Problem solving continued	All		Room E1100
10:30	<i>Coffee</i>			APS Gallery
11:00	Tutorials and Problem solving continued	All		Room E1100
12:00	Final remarks	N. Sanishvili R. Keegan G. Murshudov		Room E1100
12:30	<i>Lunch</i>			APS Gallery
1:30	End of workshop and departure			