Reproducible Science and Modern Scientific Software Development

13th eVITA Winter School in eScience sponsored by **W Norges forskningsråd** Dr. Holms Hotel, Geilo, Norway January 20-25, 2013

Welcome & Introduction

Dr. André R. Brodtkorb, Research Scientist SINTEF ICT, Dept. of Appl. Math.



Acknowledgements

- The Winter School in eScience is sponsored by

 Norges forskningsråd
- Knut-Andreas Lie, Hans Petter Langtangen, and Randall J. Leveque have helped shape the contents of this winter school.



About the Winter School

- Organized since 2001
 - Knut-Andreas Lie organizer from 2001-2012
 - André R. Brodtkorb co-organizer since 2011
- Held annually the third week in January at Dr. Holms Hotel, Geilo
- Typical schedule consists of 14 double lectures (1.5 hours) divided amongst different speakers

	Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	
07:00 - 09:00		Breakfast					
09:00 - 10:30		Lecture	Lecture	Lecture	Lecture	Lecture	
10:30 - 12:30		Brook (lunc	Break (lunch 12:30 - 14:00)				
12:30 - 14:45		DI SOK (turic					
15:00 - 16:30		Lecture	Lecture	Lecture	Lecture		
16:30 - 17:00		Coffee					
17:00 - 18:30	Lecture	Lecture	Lecture	Lecture / Poster	Lecture		









About the Winter School



- Funded by the Research Council of Norway through a series of projects
 - Winter schools in computational mathematics (2001-2004)
 - Winter schools in computational mathematics (2005-2006)
 - National Arena in eScience (2007-2010)
 - eVita Winter School (2011-2015)
- The winter school is a place to learn something new and to meet fellow researchers
 - A long break for skiing and socializng in the middle of the day
 - Typically a three course meal served every day
 - Use this opportunity to socialize and meet interesting contacts
- The lectures targets Ph.D. level students and young researchers
 - The start of the school should give an introduction that all can follow
 - The school should gradually introduce more advanced topics towards the end



Winter school topics

- 2001 Beowulf Clusters
- 2002 Computational Methods for Fluid Mechanics
- 2003 Numerical methods for nonlinear partial differential equations and Level set methods
- 2004 Adaptive methods for PDEs
- 2005 Invers problems and parameter identification for PDE models
- 2006 Automating the finite element method and turbulent flow simulation
- 2007 Monte Carlo methods
- 2008 Parallel Computing
- 2009 Optimization
- 2010 Automatic Differentiation
- 2011 Mathematical and numerical methods for multiscale problems
- 2012 Continuum Mechanics
- 2013 Reproducible Science And Modern Scientific Software
- 2014 –
- 2015 -



2012 Winter School

My own effort in following lectures has been 3,71 substantial I knew a lot about the school topic before attending 3,14 the school. I would recommend the winter school to others. 4,48 The winter school is a good place to meet scientific 4,18 peers. The winter school is a good place to learn something 4,45 new. The poster session was good, and I would like to see a 4,32 poster session also next year.

Strongly

Disagree



Neutral

Strongly

Agree

Agree

Lecturers



Dr. Rasmus Benestad, Met.no



Dr. André R. Brodtkorb SINTEF ICT



Dr. Johan S. Seland SINTEF ICT



Dr. Fernando Perez, U.C. Berkeley

Winter School Program

	Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	
07:30 - 09:00			Breakfast				
09:00 - 10:30		Fernando	Johan	Fernando	Rasmus	André	
10:30 - 12:30			Break				
12:30 - 14:45			(lunch 12:30 - 14:00)				
15:00 - 16:30		Johan	Fernando	Rasmus	Johan		
16:30 - 17:00			Coffee				
17:00 - 18:30	André	Fernando	Johan	André&poster	Rasmus		
19:30			Dinner				

Lectures start on the hour, not quarter past.

Sunday

André: Introduction & overview of reproducible science

Monday

- Fernando: Robust and comprehensible scientific software
- Johan: Software testing
- Fernando: Version control

Tuesday

- Johan: Continuous integration
- Fernando: IPython for reproducible science
- Johan: Software testing lab



School Program at a glance

	Sunday	Monday	Tuesday	Wednesday	Thursday	Friday
07:30 - 09:00						
09:00 - 10:30		Fernando	Johan	Fernando	Rasmus	André
10:30 - 12:30			Br	eak		Panel
12:30 - 14:45			(lunch 12:30 - 14:00)			
15:00 - 16:30		Johan	Fernando	Rasmus	Johan	
16:30 - 17:00			Coffee			
17:00 - 18:30	André	Fernando	Johan	André&poster	Rasmus	
19:30			Dinner			

Wednesday

- Fernando: IPython and advanced python for reproducible science
- Rasmus: Introduction to verification and validation
- André: Best practices and limits of reproducible research
- Poster session

Thursday

- Rasmus: Verification and validation
- Johan: Intellectual property rights and using the cloud
- Rasmus: Verification and validation

Friday

- André: Limits on reproducible science and advanced topics
- Panel discussion



Information about Dr. Holms

- An old hotel, opened in 1909
 - They even have their own hotel ghost, the Grey Lady.
- Meals
 - Breakfast from 7:30 to 9:00
 - Lunch from 12:30 to 14:00
 - Dinner at 19:30
 - Coffee breaks with light snacks
 - Please: no ski boots, shorts, sandals etc. ©
- Use the meals and breaks as an opportunity to meet someone new
- All beverages must be paid for separately



Dr. Ingebrikt Christian Holm



Ghost Woman, Nelson Soucasaux



Information about Dr. Holms

- Discounted ski passes can be bought at the reception
 - 3 hours for 170 NOK (50 NOK for a keycard)
- Ski and snow rentals also at a discount
 - 50% discount mid-week
- You may eat lunch in the slopes:
 - ask for a coupon at the reception before 10:00 AM
- Bowl & Dine with bowling hall
 - 50 meters to the left of the main entrance
- Swimming pool
- Spa department open for reservations









Weather Forecast

This morning:

Monday 21 January	Tuesday 22 January	Wednesday 23 January	Thursday 24 January	Friday 25 January
*	*	<i>(23)</i>	*	
-16°	-19°	-11°	-15°	-16°
0 mm precipitation per 24 hours				
1	7	\	`\	←

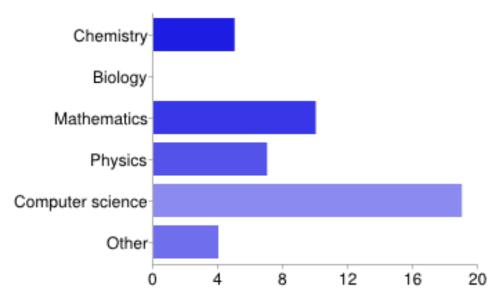
This afternoon:

Monday 21 January	Tuesday 22 January	Wednesday 23 January	Thursday 24 January	Friday 25 January
*	*	*	*	<i>(23)</i>
-16°	-19°	-11°	-15°	-14°
0 mm precipitation per 24 hours				
1	7	→	→	→



Information about participants

What are your fields of research?



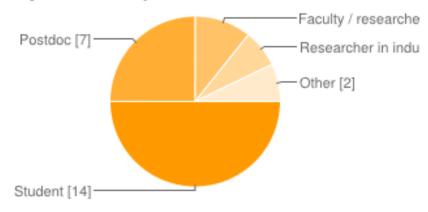
18%
0%
36%
25%
68%
14%

People may select more than one checkbox, so percentages may add up to more than 100%.



Information about participants

What is your main occupation?



Student	14	50%
Postdoc	7	25%
Faculty / researcher in academia	3	11%
Researcher in industry	2	7%
Other	2	7%



Internet

Network name: Dr. Holms Hotel

Username:

Password



Please don't use your laptop or cell phone during talks!





