

Quantum Monte Carlo in the Apuan Alps VIII



International Workshop
Saturday 27th July - Saturday 3rd August 2013
The Apuan Alps Centre for Physics @ TTI, Vallico Sotto, Tuscany

www.vallico.net/tti/tti.html

This is the programme document for the 2013 international workshop *Quantum Monte Carlo in the Apuan Alps* - the eighth such event to be held on this topic at TTI. The general purpose of workshops at this venue is to gather together limited numbers of expert physicists to discuss topics of mutual interest in greater depth than is normally possible. The focus of this meeting will be on the quantum Monte Carlo (QMC) method and other related techniques in computational electronic structure theory, and their use in understanding the quantum-mechanical behaviour of atoms, molecules, and various kinds of condensed matter.

For many types of problem the accuracy of quantum Monte Carlo is much better than that of the more widely-used density functional theory, and its scaling with number of atoms is much more favourable than that of high-level quantum chemistry. Unlike most other methods, it is also fully capable of exploiting the full power of the largest computers in the world. All topics related to applications of QMC and/or theory and algorithm development will be welcome, though it is expected that broader topics in the general area will also be discussed.

This year's meeting also has a special theme, concentrating on the relationship between QMC and density functional theory. In particular, we hope to look towards obtaining a better understanding of the relative benefits of QMC/DFT in systems and situations where DFT often fails, such as in weakly-interacting systems, strongly-correlated materials, metal-insulator transitions, magnetic properties, and biological systems. Furthermore, it is intended to look into the better integration of DFT and QMC codes. In industrial applications, where users typically require ease-of-use and a graphical user interface, how can we move towards a situation where the user may do e.g. pre-screening of candidate structures with the faster DFT, then press a 'Make the Answer Better button' which feeds the relevant wave function files into a QMC programme and spits out reliably accurate energetics for the selected problems. It is also of interest to understand how to 'move the atoms' in QMC i.e. how to exploit the power of QMC in cheaper DFT and classical-force-field molecular dynamics calculations (in the context of 'embedding methods' or otherwise). Additionally we can look at how to use QMC to develop better exchange-correlation functionals for use in DFT. Given the special nature of the meeting, we therefore warmly encourage applications to attend from DFT people who may never have run a QMC simulation in their lives but are nevertheless interested in the topic. Suggestions for alternative discussion topics and other proposals are welcome.

The format of TTI workshops is intended to encourage a relaxed and intellectually-stimulating atmosphere rather different to the usual 8am to 7pm grind of your regular conference. Formal talks are restricted to the mornings, and participants are given the freedom and space to think and to contemplate and discuss the issues at hand. Healthy recreational activities such as mountain walks are to be organized in the afternoons, and it is hoped that by taking part in these whilst breathing the clean air of the Apuan Alps and sampling local Tuscan food, the participant will be able to return home mentally and physically refreshed as well as having deepened their understanding of science.

1 LIST OF REGISTERED PARTICIPANTS - others to be added

Dario Alfè	UCL, London, U.K.	d.alfè at ucl.ac.uk
Alberto Ambrosetti	Fritz-Haber-Institut, Berlin, Germany	ambrosetti at fhi-berlin.mpg.de
Sam Azadi	Imperial College, London, U.K.	s.azadi at imperial.ac.uk
Anouar Benali	Argonne National Laboratory, U.S.A.	abenali at alcf.anl.gov
Dario Bressanini	Università dell'Insubria, Italy	dario.bressanini at uninsubria.it
Pascal Bugnion	University of Cambridge, U.K.	pob24 at cam.ac.uk
Mauro Causà	University of Napoli, Italy	mauro.causa at unina.it
Gareth Conduit	University of Cambridge, U.K.	gjc29 at cam.ac.uk
Mike Deible	University of Pittsburgh, U.S.A.	mjd87 at pitt.edu
Andrea Droghetti	Trinity College, Dublin, Ireland	drogheta at tcd.ie
Neil Drummond	Lancaster University, U.K.	n.drummond at lancaster.ac.uk
Edgar Engel	University of Cambridge, U.K.	eae32 at cam.ac.uk
Elif Ertekin	University of Illinois, U.S.A.	ertekin at illinois.edu
Matthew Foulkes	Imperial College, London, U.K.	wmc.foulkes at imperial.ac.uk
Mike Gillan	University College, London, U.K.	m.gillan at ucl.ac.uk
Richard Hennig	Cornell University, U.S.A.	rhennig at cornell.edu
Kenta Hongo	JAIST, Japan	kenta_hongo at mac.com
Ken Jordan	University of Pittsburgh, U.S.A.	jordan at imap.pitt.edu
Jonathan Lloyd-Williams	University of Cambridge, U.K.	jhl50 at cam.ac.uk
Pierre-Francois Loos	Australian National University	loos at rsc.anu.edu.au
Matthew Lyle	University of Cambridge, U.K.	mjl78 at cam.ac.uk
Martin Krupicka	Max Planck Institute, Mulheim	martin at bhpromo.cz
Ryo Maezono	JAIST, Japan	rmaezono at mac.com
Natalia Matveeva	University of Trento, Italy	matveeva.na at gmail.com
Bartomeu Monserrat-Sanchez	University of Cambridge, U.K.	bm418 at cam.ac.uk
Elaheh Mostaani (V)	University of Lancaster, U.K.	emostaani at gmail.com
Tim Mueller	John Hopkins University, Baltimore, U.S.A.	tmueller at jhu.edu
Richard Needs	University of Cambridge, U.K.	rn11 at cam.ac.uk
Joshua Schiller	University of Illinois, U.S.A.	jschiller90 at gmail.com
Luke Shulenburg	Sandia National Laboratory, U.S.A.	lshulen at sandia.gov
James Spencer	Imperial College, U.K.	j.spencer at imperial.ac.uk
Jian Sun	University of Cambridge, U.K.	js2065 at cam.ac.uk
Alex Thom	University of Cambridge, U.K.	ajwt3 at cam.ac.uk
Alexandre Tkatchenko	Fritz-Haber-Institut, Berlin, Germany	tkatchen at fhi-berlin.mpg.de
Mike Towler	University of Cambridge/UCL, U.K.	mdt26 at cam.ac.uk
Peter Townsend	University of Cambridge, U.K.	psmt2 at cam.ac.uk
Tack Uyeda	JAIST, Japan	tueeeda at jaist.ac.jp
Will Vigor	Imperial College, London, U.K.	w.vigor11 at imperial.ac.uk
Anatole von Lilienfeld	Argonne National Lab, U.S.A.	anatole at alcf.anl.gov
Lucas Wagner	University of Illinois, U.S.A.	lkwagner at illinois.edu

FAMILY MEMBERS

Frida Tkatchenko (V)

STAFF

Samantha Keil, Saska Towler, Jamie Towler

Lisa Johnson-Davies

2 FLIGHTS AND TRANSPORT

This section gives details on how to get to the Institute for people flying into our recommended airport: Galileo Galilei Airport, Pisa. It is also possible to fly to Florence which is only slightly further away - though flights to this airport are limited. In principle one could also fly to other airports such as Perugia, Bologna, Ancona, Parma, Milano, Verona, Genova or Roma but you should count on a train ride of up to four or five hours to get to the Institute (we can arrange this for you). A list of airlines flying to Pisa from

destinations within Europe is given on the TTI web page (see 'Flying to Italy' in the left-hand column). Americans should note that Delta Airlines now operate a direct service to Pisa from New York. Further details about transport, including how to drive to the Institute, are also given on the TTI web site.

Participants should aim to arrive at Pisa airport on Saturday 27th July (Cambridge people on Friday 26th). If this is not possible (e.g. if flights from your country are irregular) then we recommend having a brief holiday in Florence or similar before coming to TTI (or you could always volunteer to arrive early and help with the vast amount of back-breaking labour required to set up the conference!). Please note that late departures are not encouraged because of the summer school taking place immediately after the workshop (as well as transporting people to airports and so on we need to reboot the entire village and clean everything in less than a day).

How to get to TTI from Pisa airport on Saturday 27th July:

Go to Pisa Centrale train station. The best way to do this from the airport is by taxi (costs around 9 EUR) - you should see the taxi rank as soon as you exit the terminal building. The *stazione* (phonetic: 'statsionay ferrovia') is a 5-minute journey. If the taxis are on strike or you are desperate to save a few Euros you could alternatively take a short train ride from Pisa Aeroporto station (which you get to by walking out of one end of the terminal building - turn left as you walk into the main hall) or you could - presumably - take a bus. Once at Pisa Centrale station you then need to get a train to Barga-Galliciano. This is an isolated station north of the city of Lucca somewhere along a branch line going up the valley of the river Serchio into the mountains (see the map on the TTI web site). Depending on the train time, you may need to change at Lucca to get the train north. The train will usually be flagged as going to "Aulla-Lunigiana", "Minucciano", "Piazza al Serchio" or "Fivizzano". See the printed timetables on the station wall to check where each train stops, and the electronic screens for the departure platform. Note that in Italian, Departures is 'Partenze', and Arrivals is 'Arrivi' - make sure you're looking at the right timetable or screen.

The train in question is a little unimportant train, and for some reason only tickets for big important trains seem to be available on the internet. It is easy to buy tickets on the station platform either from a human ("Uno a Barga-Galliciano. Solo andata.") or from one of the ticket machines (which can be requested to speak English). On all Italian train journeys you are supposed to validate ('convalidare') your ticket by inserting it into one of the small wall-mounted green and white machines in the station or you may have to pay a fine - though I have never seen a ticket inspector on any of the trains that you will take. Note that Italian trains are very (even absurdly) cheap by international standards, particularly British ones. The ticket should cost around 4 to 6 Euros.

One final thing that has caused confusion in the past: at Lucca and Pisa some of the trains leave from a platform ('binario') labelled '1TO' or '1TE', meaning 1 Tronco Ovest (west) and 1 Tronco Est (east). This is *not the same* as Platform 1. All the 'through platforms' are labelled 1, 2, 3 etc., and 1TO and 1TE refer to separate 'terminus platforms' which you can find by walking to either the west or east end of Platform 1.

At Barga-Galliciano station you should find a TTI representative who will meet each Saturday train as required and take new arrivals to the Institute. If no-one is there you can wait in the station café - do call if you have to wait more than five or ten minutes. Clearly we need to know in advance the time of the train on which you intend to arrive. The timetable is linked from the TTI web site, but all Saturday train times are in fact given in the table below. Note that the last train from Pisa is around 20:50 so it would be a good idea to arrive earlier in the day if possible (particularly if you want to enjoy the welcome buffet dinner at 19:30 - remember that staff members who have to pick up latecomers miss their dinner too!).

In emergencies it is possible to get a taxi to Vallico Sotto from the station but in general this needs to be pre-booked - see the instructions on the web site (Barga Taxi : bargataxi@libero.it Tel. 331 3378051 or 339 5678336). If you are a non-Italian speaker who hasn't pre-booked and you need to talk to the guy (Massimo) on the phone you will find he doesn't speak English so just say (phonetic) "Taxi a Vallico Sotto da la stasjonay di Barga-Gallicano?" or similar down a phone at him - the trip should cost around

35 Euro. Note that “I don’t speak Italian” is “Non parlo italiano.”

In case of problems contact Mike on his mobile - 00 44 7432 491113. (Additional emergency assistance may be available from Samantha Keil on 00 44 7979 554034, though be aware that she doesn’t know where anything is geographically. She does, however, generally know where Mike is, which is kind of the point). TTI has two direct phone lines (0583 761608 and 0583 1805441) which you should use as a last resort, since it is unlikely anyone useful will be near them.

3 TRAIN TIMETABLES

See www.trenitalia.com and click the British flag at the top right.

Saturday 27th July, Pisa Centrale to Barga-Gallicano station

dep. Pisa	arr. Lucca	dep. Lucca	arr. Barga-Gallicano
05:25			06:52
06:13	06:39	06:56	07:37
07:50			09:15
10:20	10:47	11:30	12:12
12:50	13:17	13:26	14:14
13:43			14:53
15:20			16:31
16:20	16:44	16:56	17:44
17:50			19:00
18:50			20:27
19:50			21:31
20:50	21:17	21:40	22:20

Saturday 3rd August, Barga-Gallicano to Pisa Centrale station

dep. Barga-G.	arr. Lucca	dep. Lucca	arr. Pisa
05:56	06:40	06:52	07:16
06:39			08:13
07:24	08:11	08:42	09:13
08:43	09:25	09:42	10:13
12:00	12:50	13:12	13:43
14:04			15:43
15:18	16:05	16:12	16:43
18:49	19:37	19:42	20:13
20:16			22:13

3.1 From Milano

People coming from more distant countries often only have a choice of coming to Milano airport. Here is a summary of advice for them.

Travel from Milano Malpensa airport to Milano Centrale train station:

The Malpensa Express train departs from Terminal 1 for Milano Centrale train station around twice an hour. (One can also get to other Milano stations Cadorna, Bovisa and Saronno but Centrale is the main train station where you need to catch onward trains. Note that the Malpensa-Centrale line only opened in 2010 so you may still encounter outdated advice that you need to travel to Cadorna from the airport). The first train departs Malpensa at 05.43, the last train departs 22.43. Journey time is around 40-50 minutes.

Fare: 10 Euro one-way - don't get in a taxi as it will cost you 65+ Euro.

Travel from Milano Linate airport to Milano Centrale train station:

This smaller airport is much closer to the centre than Malpensa, and therefore it is feasible to use buses or taxis to get to the train station. See the Linate Airport section of wikitravel.org/en/Milan for details about the various options.

From Milano Centrale train station to Barga-Gallicano

Saturday 27th July 2013

From Milano Centrale as above. Then choose one of the following trains - the 08:10 and 13:10 are probably best since there is only one change, and no later train will get you to Vallico Sotto in time for dinner. (There are other possibilities, but they involve tricky 4 train connections, or getting up too early).

OPTION 1 - (from 24.70 EUR) *** - BEST

Milano Centrale	08:10	--> Pisa Centrale	12:21
Pisa Centrale	13:43	--> Barga-Gallicano	14:53

OPTION 2 - (from 34.70 EUR) *** - SECOND BEST

Milano Centrale	13:10	--> Pisa Centrale	16:57
Pisa Centrale	17:50	--> Barga-Gallicano	19:00

OPTION 3 (from 16 EUR)

Milano Centrale	14:05	--> La Spezia Centrale	17:19
La Spezia Centrale	17:29	--> Aulla Lunigiana	17:53
Aulla Lunigiana	19:02	--> Barga-Gallicano	20:15

OPTION 4 (from 14.70 EUR)

Milano Centrale	16:05	--> Viareggio	19:58
Viareggio	20:10	--> Lucca	20:27
Lucca	20:44	--> Barga-Gallicano	21:31

If you fly into Milano before Saturday, another option is to stay in a suitable hotel in Milano and take a train the day after.

Before you arrive, write down the details of suitable hotels near the station. There is a good site where you can book these and print out maps at:

<http://www.traveleurope.it/milano.htm>

or better still:

http://www.traveleurope.it/milan/milan_central_station.shtml

The Hotel Monopole seems a good one to me (prices from 60 EUR)

4 SPECIFIC TRAVEL PLANS

Gareth Conduit, Jonathan Lloyd Williams, Bartomeu Monserrat-Sanchez, Edgar Engel
Arr Pisa 09:45 Wed 24 July. Trip to Rome. Drive rental car to TTI Fri 26 July
Dep Pisa 22:15 Sat 3 Aug

Pascal Bugnion
Arr Pisa Centrale Fri 26 July 14:28. Meet Conduit car and travel to TTI
Dep Pisa Centrale Sat 3 Aug 13:32

Peter Townsend
Train to Pisa. Train dep Pisa 13:43 arr Barga-Gallicano 14:53
Train dep Barga-Gallicano Fri 2 August

Lisa Johnson-Davies
Arr Pisa Fri 26 July 14:50. Train dep Pisa 16:20 arr Barga-Gallicano 17:44
Dep Pisa Sun 11 Aug 16:30

Matthew Foulkes
Arr Pisa Fri 26 July 15:10. Train dep Pisa 16:20 arr Barga-Gallicano 17:44
Dep Pisa Fri 2 Aug 15:45

Sam Azadi
Arr by train from Trieste to Barga-Gallicano Fri 26 July 19:00
Dep Bergamo Sat 3 Aug 17:15

Andrea Droghetti
Arr by train Sat 27 July Barga-Gallicano 11:59 (PICK UP AT 12:12)
Dep Fri 2 Aug by train

Ken Jordan, Mike Deible
Arr Pisa Sat 27 July 07:05. Train dep Pisa 10:20 arr Barga-Gallicano 12:12
Dep Sat 3 August for Pisa (hotel), fly from Pisa Sun 4 August 10:00

Mike Gillan
Arr Pisa Sat 27 July 09:30. Train dep Pisa 10:20 arr Barga-Gallicano 12:12
Dep Pisa Fri 2 Aug pm

Martin Krupicka
Arr Pisa Thu 1 Aug. Train arr Barga-Gallicano 17:25 (TAXI BOOKED)
Dep Firenze Mon 12 Aug 17:00

James Spencer
Arr Pisa 09:45 Sat 27 July. Train dep Pisa 12:50 arr Barga-Gallicano 14:14
(PICKUP AT 14:53)
Dep Pisa 19:20 Sat 3 Aug

Alex Thom, William Vigor
Arr Pisa Sat 27 July 09:45. Train dep Pisa 13:43 arr Barga-Gallicano 14:53
Dep Pisa Sat 3 Aug 17:20

Alberto Ambrosetti
Arr Pisa Sat 27 July 12:45. Train dep Pisa 15:20 arr Barga-Gallicano 16:31
(PICKUP AT 17:44)
Dep Pisa Sat 3 Aug 13:20

Natalia Matveeva
Arr by train from Trento Sat 27 July to Barga-Gallicano 17:44
Dep by train Sat 3 Aug from Barga-Galliano 08:43

Luke Shulenburg
Arr Roma Sat 27 July 09:25. Train dep Roma Term. 13:29 arr Barga-Gallicano 17:44
Dep Pisa Centrale 09:00 Sat 3 Aug to Roma for flight Sun 4 Aug

Richard Needs, Jian Sun, Matthew Lyle
Arr Pisa Sat 27 July 18:55. Train dep Pisa 19:50 arr Barga-Gallicano 21:31
(PICK UP AT 22:20)
Dep Pisa Sat 3 Aug 19:20

Pierre-Francois Loos
Arr Pisa Sat 27 July 18:45. Train dep Pisa 19:50 arr Barga-Gallicano 21:31
(PICK UP AT 22:20)
Dep Pisa Fri 2 Aug 13:50

Elaheh Mostaani
Arr Pisa Sat 27 July 19:35. Train dep Pisa 20:50 arr Barga-Gallicano 22:20
Dep Pisa Sun 11 Aug 11:50

Tim Mueller
Arr Pisa 07:00 Sat 27 July. Drive rental car to TTI.
Dep Pisa 09:50 Sat 3 Aug

Anatole von Lilienfeld
Arr Basel beginning July. Drive rental car to TTI with Benali Sat 27 July
Dep Sun 4 Aug am by car car

Anouar Benali
Arr with von Lilienfeld in rental car Sat 27 July.
Dep Pisa Sat 3 Aug 13:20

Dario Alfe
Arr by car Sat 27 July pm
Dep by car Tue 30 July pm

Richard Hennig
Arr by car Sat 27 July pm
Dep by car Wed 31 July am

Alexandre Tkatchenko, Frida Tkatchenko
Arr by car Sat 27 July pm
Dep by car Sat 3 Aug pm

Mauro Causa
Arr by motorbike Sat 27 July pm
Dep by motorbike Fri 2 Aug pm

Ryo Maezono, Kenta Hongo, Tack Uyeda
Arr Pisa Fri 26 July (hotel). Drive rental car to TTI Sat 27 July
Dep Fri 2 August for Pisa (hotel), fly from Pisa Sat 3 Aug

Lucas Wagner, Elif Ertekin, Joshua Schiller
Arr Pisa Sat 27 July 07:00. Drive rental car to TTI.
Dep Pisa Sat 3 Aug

Neil Drummond
Arr Roma 13:20 Tue 30 July. Train dep Roma Term. 15:59 arr Barga-Gallicano 21:31
TAXI BOOKED.
Dep Pisa 15:15 Fri 9 Aug (Train dep Barga-Gallicano 08:43)

Dario Bressanini
Will arrive and depart in own car. Dates uncertain.

5 ACCOMMODATION

TTI, ATTIC - one single mattress
Mike Towler

TTI, NURSERY - one single bed
Richard Needs

TTI, PLAYROOM - two single beds, one double bed
Mauro Causa, Sam Azadi, Bartomeu Monserrat-Sanchez

TTI, PINK ROOM
Samantha Keil, Saska Towler, Jamie Towler

TTI, LILAC ROOM - two single beds
Natalia Matveeva, Lisa Johnson-Davies

TTI, TINY ROOM - one single bed
Dario Alfe (from Sat 27 - 3 nights)
Neil Drummond (from Tue 30)

TTI, RED ROOM - one double bed
Matthew Foulkes

TTI GARDEN ROOM - two single beds (bunk)
Jonathan Lloyd-Williams, Peter Townsend

DOCTOR'S HOUSE, UPPER FAR ROOM - one double bed
Alexandre Tkatchenko, Frida Tkatchenko

DOCTOR'S HOUSE, UPPER MIDDLE ROOM - two single beds
Pierre-Francois Loos, Tim Mueller

DOCTOR'S HOUSE, UPPER NEAR ROOM - one double bed
Mike Gillan

DOCTOR'S HOUSE, LOWER APARTMENT - one double bed, two single bunk beds
Mike Deible, Will Vigor, Jian Sun

CASA GIANPIERO - ROOM 1 - one double bed
Ken Jordan

CASA GIANPIERO - ROOM 2 - two single beds

Luke Shulenburger, Andrea Droghetti

CASA FRANCA - ROOM 1 - 1 double bed
Alberto Ambrosetti

CASA FRANCA - ROOM 2 - 1 double bed
Dario Bressanini

CASA FRANCA - ROOM 3 - 1 double bed
Alex Thom

CASA FRANCA - ATTIC ROOM - 1 single bed
Tack Uyeda

CASA LUCIANA - ROOM 1 - 1 single bed
Anouar Benali

CASA LUCIANA - ROOM 2 - 1 double bed
Anatole von Lilienfeld (switch to BEDOUIN TENT for night of Sat 3 Aug)

CASA SARDA - 1 single bed
Elaheh Mostaani

CASA LONTANA - ROOM 1 - 1 double bed, 1 single bed
Pascal Bugnion, Joshua Schiller

CASA LONTANA - ROOM 2 - 1 double bed
Martin Krupicka

CASA LONTANA - ROOM 3 - 1 single bed
Richard Hennig

BEDOUIN TENT (www.vallico.net/tti/tti_tent.html)
Edgar Engel, Gareth Conduit, Matthew Lyle
Anatole von Lilienfeld (for night of Sat 3 Aug)

DA SANDRA (multiple commercial rooms: dasandra.jimdo.com)
Local restaurant offering private rooms and apartments at a reasonable price
- 3 minute drive / 15 minute walk - more suitable for people with cars but
transport will be arranged even for people without. Please pay the owner
directly (Sandra's daughter Serena is responsible for accommodation at the
restaurant) but ask MDT to book the room. Cost : 60 Euros per night.

DA SANDRA - ROOM 1 - 1 double bed
James Spencer

DA SANDRA - ROOM 1 - 1 double bed
Unavailable

DA SANDRA - APARTMENT 1 - 1 double bed
Ryo Maezono

DA SANDRA - APARTMENT 1 - 1 double bed
Kenta Hongo

DA SANDRA - APARTMENT 1 - 1 double bed

Lucas Wagner, Elif Ertekin

CASALE DEI RUSCELLI (www.casaledeiruscelli.com)

Posh apartments for rich people requiring privacy - 12 min drive - car and extra payment required. Please pay the owner directly - but ask MDT to book this.

6 CONFERENCE VEHICLES

Max 46 people to transport simultaneously; 58 official seats
plus 10 temporary.

OFFICIAL VEHICLES

17-seater bus - driver: Mike Towler
9-seater rental car - driver: Tim Mueller
6-seater Fiat Multipla - driver: Martin Krupicka

PRIVATE VEHICLES

5-seater rental car - driver: Ryo Maezono
5-seater rental car - driver: Lucas Wagner
5-seater rental car - driver: Edward Engel
5-seater rental car - driver: Anatole von Lilienfeld
5-seater rental car - driver: Alexandre Tkatchenko
1-seater motorbike - driver: Mauro Causa

OTHER PRIVATE VEHICLES PRESENT FOR PART OF THE WEEK:

5-seater rental car - driver: Richard Hennig (Sat - Wed)
5-seater rental car - driver: Dario Alfe (Sat - Tue)

SPARE DRIVER (please bring driving license)

Sam Azadi

7 THINGS TO BRING WITH YOU

- The slides for your talk if you intend to give one - see later section for supported formats.
- Your laptop, if you wish (though this is completely not necessary, as we have large numbers of them - see note in Technical Equipment section). Note that our official laptops are now starting to die - we have lost 5 of them to electronic failures in the last year alone - and we no longer have funds to replace them. So if you have old laptops you would like to donate to the Institute these would be very welcome (particularly for the associated QMC summer schools).
- Summer hiking gear such as boots, socks, little rucsacs, sunhats etc.
- Italian plug converters if you want to plug anything in (we have some spare but donations of these are gratefully accepted). Our sockets mostly have two round pins (with an optional third one between them). There are two types of thin prongs on European adaptors. You want the thinner of the two. Just to confuse things, there are also lots of totally incompatible English plug sockets into which English equipment can be plugged directly.
- Some Euros for spending in restaurants and shops (minimum 25 Euros per day). Please note that there is no easily accessible cash machine near the Institute, and although we might pass them from time to time on our afternoon trips, large numbers of people getting money out can cause considerable delays. There is a cash machine in Pisa airport to your left as you emerge into the arrivals hall (look under the escalator leading to the upper level). Go up the escalator to find an alternative cash machine if that one isn't working. A few years ago a cash machine was in fact

setup in Fabbriche di Vallico a few kilometres away from the Institute - this is now much less flaky than when it was first installed but relying upon it to actually give you money would not be sensible.

- People who intend to visit caves or canyons should bring some clothes and old shoes that you don't mind getting wet.
- Climbing/caving equipment (harness, boots, helmet, via ferrata 'absorber', head torch) if you intend to take part in such activities and already have some (don't buy them just for this trip). We have a fair amount of gear we can lend but not enough for everyone.
- Light sleeping bag and a torch (if you intend to sleep in the Bedouin tent).
- Hay fever tablets. Some people who have lived in darkened basements in huge cities most of their lives sometimes have difficulty with pollen when they come to live in the countryside.
- A musical instrument, if you can play a portable one. See Section 15.
- Sunscreen. It is likely to be quite hot in the first week of August, but note that because we are in the mountains occasional afternoon rain showers are not unknown.
- A towel
- Swimming costume (if you wish to go swimming).
- Earplugs - if you are sharing a room - to avoid being disturbed by snoring people.

In the tradition of earlier workshops, you might also optionally like to bring

- A nice bottle of wine (or whatever passes for it in your country).
- An interesting thing

8 CONFERENCE SCHEDULE

This section contains the schedule for the conference, including a list of talks. The number of talks per day is deliberately small to allow time for thinking, discussion and deliberation. In principle there could be evening discussion sessions if required. If you do not wish to give a talk, or if you wish to give a shorter/longer talk than suggested, please ask. All excursions and activities are, of course, optional - and you may elect simply to relax at the Institute in the afternoons - though then transport to the evening restaurant will need to be arranged. I have to book restaurants well in advance for such large groups so please make it known as soon as you can if you do not wish to attend particular meals.

Friday 26th July

EARLY ARRIVALS

Erection of Bedouin Tent by its inhabitants + MDT

DINNER: Canapale (Vallico Sopra) - TO BOOK FOR 13 PEOPLE

Saturday 27th July

ARRIVALS

7pm : Welcome buffet dinner and drinks in the Institute garden (45 people)

Sunday 28th July

- 8.30am : Mike Towler (5 minutes)
 - "Welcome to Tuscany"
- 8.35am : Mike Gillan (50 minutes)
 - "Quantum Monte Carlo benchmarks for weak non-covalent interactions"
- 9.30am : Dario Alfe (25 minutes)
 - "Graphene on Ir(111): growth and thermodynamics from combined experimental and theoretical methods"
- 10.00am : Ken Jordan (50 minutes)
 - "Quantum Monte Carlo studies of correlation-bound anions and of organic diradicals"
- 11.00am : Matthew Foulkes (50 minutes)
 - "Forces and correlated sampling in DMC"
- 12.00am : Anouar Benali (25 minutes)
 - "Quantum Monte Carlo calculations of many-body van der Waals forces in rare gas crystals and biomolecules"
- 12.30pm : CHURCH (if you want)

POSSIBLE EXCURSIONS:

Trip to Alto Matanna. Numerous spectacular walks of varying difficulty. See the Versilia coast, Elba, Corsica and sometimes even France from the easily accessible summits of some of the more beautiful scenery in the Apuan Alps. Bring one of the Institute's antique telescopes to watch the more courageous of you scale the 500 foot cylindrical barrel of Monte Procinto. Followed by drinks and dinner in 19th Century Alpine hotel.

- Balloon station walk (short and easy)
- Monte Matanna walk (medium) possible extended to Monte Nona.
- Monte Procinto climb (strenuous)
- Monte Croce circular walk from Palagnana (strenuous)
- Grotta all'Onda walk (Neanderthal cave) (very strenuous)

DINNER : Matanna (BOOKED FOR 45)

Monday 29th July

-
- 8.30am : Alexandre Tkatchenko (50 minutes)
 - "Explicit many-body van der Waals corrections to DFT, and how QMC can help to develop them"
- 9.30am : Luke Shulenburger (50 minutes)
 - "Status of DMC for condensed phases"
- 10.30am : Lucas Wagner (50 minutes)
 - "Can we understand the high-Tc superconducting cuprates from first principles?"
- 11.30am : Ryo Maezono (25 minutes)
 - "Studies of electron-hole systems using DMC"
- 12.00am : Sam Azadi (25 minutes)
 - "Quantum Monte Carlo study of high-pressure solid hydrogen"

POSSIBLE EXCURSIONS:

- Walk Matanna to Monte Forato (rock arch) to Fornovolasco - new ferrata route Tana che urla cave
- Walk Palagnana-Monte Croce-Fornovolasco
- San Pellegrinetto Walk led by Mountain Guide Saska Towler
- Grotta del Vento tourist cave
- Fornovolasco church and flood frescoes
- Independent cave-hunting (ask Mike)
- Swimming at Barga

- Staying in the monastery
DINNER : New Eremo di Calomini (BOOKED FOR 44)

Tuesday 30th July

8.30am : Tim Mueller (50 minutes)
- "Quantum Monte Carlo for materials design"
9.30am : Gareth Conduit (50 minutes)
- "Concurrent materials design"
10.30am : Richard Hennig (50 minutes)
- "Computational discovery and design of materials for energy technologies and electronic devices"
11.30am : Mauro Causa (25 minutes)
- "Correlated maximum probability domains in crystals"
12.00am : Elif Ertekin (25 minutes)
- "QMC for point defects in semiconductors and wide-band gap oxides"
12.30am : Tack Uyeda (15 minutes)
- "Ohmic contact on diamond semiconductors"

A DAY IN THE VILLAGE

- Relaxing, sunbathing, reading, studying, discussing

POSSIBLE EXCURSIONS:

- Circular walk from Vallico via San Luigi and Pian di Lago to the Trassilico fortress and back via the landslide.
- Turrite di San Rocco canyon walk
- Independent cave-hunting (ask Mike)
- Boating on the Turrite Cava lake (+ Buca del Lago della Turrite Cava)

DINNER : Da Sandra (BOOKED FOR 44) - CANCELLED DUE TO SANDRA ILLNESS

Instead eat at the Vallico Sopra Festival.. Mike to arrange.

Wednesday 31st July

8.30am : Anatole von Lilienfeld (50 minutes)
- "Preaching on first principles views on chemical compound space, atom centered potentials, and statistical learning"
9.30am : Alex Thom (50 minutes)
- "Linked stochastic coupled cluster theory"
10.30am : Bartomeu Monserrat-Sanchez (50 minutes)
- "White dwarf cooling: electron-phonon coupling and the metallization of solid helium"
11.30am : William Vigor (25 minutes)
- "Accelerating Full Configuration Interaction Quantum Monte Carlo"
12.00am : Alberto Ambrosetti (25 minutes)
- "Long range correlation energy from isotropically damped Quantum harmonic oscillators"

POSSIBLE EXCURSIONS:

- Monte Sumbra
- Coreglia di Antelminelli and Buca delle Fate
- Swimming and shopping in Bagni di Lucca
- Staying in the monastery

DINNER : Il Totto, Sassi (BOOKED FOR 44)

Thursday 1st August

-
- 8.30am : James Spencer (25 minutes)
 - "A mysterious talk about an unknown yet topical subject"
- 9.00am : Matthew Lyle (50 minutes)
 - "Low density nanocrystalline alumina"
- 10.00am : Ken Jordan (25 minutes)
 - "Proton disorder in ice"
- 10.30am : Pascal Bugnion (50 minutes)
 - "Spins, superfluidity, and ultracold atomic gases"
- 11.30am : Pierre-Francois Loos (25 minutes)
 - "Uniform electron gases: electrons on a ring"
- 12.00am : Natalia Matveeva (25 minutes)
 - "Localization of an impurity in a bilayer system of dipoles"

A DAY IN THE VILLAGE

- Relaxing, sunbathing, reading, studying, discussing
 - Metal detecting
 - Orienteering
 - Abseiling to the Buca della Fate di Vallico di Sotto
 - Football match - Vallico Sotto against the world/Vallico Sotto contro il mondo
- DINNER : Provided by Federico and friends at Vallico Sotto (BOOKD FOR 44)
- MUSICAL EVENING back at the monastery afterwards

Friday 2nd August

-
- 8.30am : Neil Drummond (50 minutes)
 - "Electronic structure of two-dimensional crystals of hexagonal boron nitride"
- 9.30am : Richard Needs (50 minutes)
 - "Decomposition and terapascal phases of water ice"
- 10.30am : Mike Deible (25 minutes)
 - "Quantum Monte Carlo studies of water clusters and water-acene complexes"
- 11.00am : Andrea Droghetti (25 minutes)
 - "A DFT+model Hamiltonian approach to zero-bias transport in nanostructures: work in progress"
- 11.30am : Kenta Hongo (25 minutes)
 - "Finite-size effects in diffusion Monte Carlo simulations of para-diiodobenzene"
- 12.00am : Elaheh Mostaani (25 minutes)
 - "Binding energy of bilayer graphene"

POSSIBLE EXCURSIONS:

- Lucca
- Orrido di Botri
- Staying in the monastery

DINNER: Il Mulino, Fabbriche di Vallico (BOOKED FOR 37)

Saturday 3rd August

DEPARTURES

Daring excursion for volunteers (total walking time approximately 5 hours).

Volunteers:

Elif Ertekin, Lucas Wagner, Joshua Schiller

POSSIBILITY 1: The Gulf of Poets

"One of the finest coastal hikes in Italy".

p. 174 in MDT's "The Alps of Tuscany" book.

Leave TTI at 7:30 am arriving at Riomaggiore c. 9.30.
Walk to Portovenere along cliff-top path via the Gulf of Poets (5 hours).
Bus to La Spezia, Train to Riomaggiore (both very frequent). Return in
time for 7pm dinner.

POSSIBILITY 2: Monte Corchia from Isola Santa

Details on request.

POSSIBILITY 3: Pizzo D'Uccello

The Matterhorn of the Apuan Alps

Details on request.

Extra unassigned activities which can be easily planned:

- Buffardello park
 - Random cave hunting trips following new cave maps
(e.g. Campolemissi, Fabbriche di Vallico, Antro della Paura, Motrone)
 - Lucca Villas
 - Pietrasanta
 - Vinci (Leonardo's birthplace)
 - Walk from Collodi to Pescia
 - Local mountain trips (Pania della croce etc..)
 - Marble quarries
 - Beach trips to e.g. Sestri Levante, Portofino, Cinque Terre, Lerici
-

9 TTI TECHNICAL EQUIPMENT

There are various modern laptop computers in the Institute available both for general use. Most dual boot into some version of OpenSuse or Ubuntu Linux and one of Windows XP/Vista/7. You may of course bring your own laptop if you wish. Please be careful of the electrics when plugging in your own machine in order to avoid shorting out the projector etc. - in fact, it's better to ask where to do so. Note that most of the available plug sockets in the lecture hall are of the *English* type though some Italian ones are available.

All internet connections are made through a standard wireless network. If you wish to bring your own laptop then it therefore needs to be wireless-enabled if you wish to log into the network (for older machines we have three spare wireless network cards that you can plug into your laptop PC card slot). The Institute SSID is 'TTI' and the network is completely unencrypted due to the total absence of hackers, or indeed computers, in remote mountain villages. Since June 2009, TTI is hooked up to the local 2 Mb/s wireless broadband network.

Apart from computers and networking devices, we also have the following equipment available:

- A HP Laserjet black and white printer (on a wireless print server, so one can print from anywhere in the Institute) - the relevant print queue is called 'hp'.
- Canon Pixma ip4000 colour inkjet printer
- Hi-Ti Transphotable and Sony photo printers for instant printing of your photographs (you can plug in your camera directly - no need to go through a laptop - accepts all memory card formats that I am aware of).
- Epson Perfection 4990 scanner
- A3 laminator
- Guillotine.
- Finepix F455 digital camera
- Four memory sticks
- A supply of writeable CD-Rs, CD-RWs and DVD-Rs.
- The usual stationery and staples etc..

There are also a very large number of scientific and technical books which may be borrowed (top floor of the main building, and in the various bookshelves in the church).

Please note that there is also a new pigeon-hole bookcase intended for printouts of 'the literature'. This has currently been set up to include all the relevant papers for '*21st-century directions in de Broglie-Bohm theory and beyond*' - a huge conference we ran a couple of years ago, but it may be refilled with anything you like. You are welcome to borrow these papers, but please put them back in the same place you got them from as they are all carefully filed..

10 INTERNET USE

TTI laptops are mainly black/grey Sony Vaios with a few red Acer Ferraris (note the difference in power supplies - the ones for the Ferraris have yellow ends, the Sony machines have black ones). Almost all are in dual boot configurations with some version of OpenSuse/Ubuntu Linux and Windows XP/Vista/7 - after turning them on you should choose which OS you want. All will boot into Linux after some time by default unless you say otherwise. We essentially never use Windows here so the setup on the Windows partitions will be minimal if it has been done at all.

Since June 2009 the monastery's local network connects to the outside world through a 2Mb/s wireless broadband network (having previously been on dialup!). All local machines have static IP addresses 192.168.1.2x (where 2x is 20 plus the number of the machine - a red plastic label saying e.g. `tti_laptop9` implies 192.168.7.29) so they can all talk to each other via ssh or ftp etc. With appropriate software all the laptops can be run as a parallel supercomputer should anyone need to do intensive calculations.

Other network details for administrators: IP 192.168.1.xx (static xx=10-99, DHCP assigned numbers from xx=102-200), Gateway 192.168.1.1, Primary DNS 62.94.0.41, Secondary DNS 212.216.112.112.. The router has a (password protected) web page at 192.168.1.2. Other equipment attached to the network: a VoIP phone (192.168.1.98), an internet radio (192.168.1.99), a wireless print server (192.168.1.101), and possibly the NEC projector on DHCP. Do not assign your own static IP number on personal hardware without consulting MDT/PLR.

Please be mindful of the needs of other users of the network. Although we have broadband, it is hardly a superfast connection, and downloading Gb of files to patch your machine or whatever is discouraged.

Note also that there is network coverage only in the main TTI building and not in any of the other houses we use for accommodation (Doctor's House, Casa Franca, Casa Gianpiero, Casa Luciana, Casa Sarda, Casa Lontana). Possibly - given its new location - the Luxury Bedouin Tent may be covered though we won't be able to test this until it's put up.

11 PRESENTATION EQUIPMENT

The church is equipped with a good quality NEC MT1075 projector and an auxiliary Toshiba DPD TDP-T250U projector with DVI and regular RGB cabling . There is a giant 16' by 12' main screen, a 7'8 x 5'9 electric auxiliary screen, an Avervision document camera, a dual projection stand, a laptop, a DVD player with decent speakers, and various wireless control devices. There is a giant blackboard in the church and a smaller one in the main corridor stolen from the TCM Seminar room in the Cavendish Laboratory. There are two blackboards outside, and a portable one which can be taken on excursions if you wish to debate physics in restaurants or up mountains.

The NEC projector is wireless capable, so you can beam your talk from your laptop straight to it from anywhere in the room, as well as with old-fashioned direct connection (technical specs on the TTI website). The Institute projection laptop - though normally bootable into either Linux or Windows - will normally be running under Windows because Linux Powerpoint viewers mostly do not display Microsoft-generated files correctly. Obviously it will accept CDs and memory sticks and have the usual software such as Acroread and Powerpoint. On balance it is probably best to bring your talk on a CD or USB device or email it to MDT beforehand and he will ensure that it is on the projection laptop ready for your talk. We would be grateful if you could leave your talk on the Desktop of this machine so that your talk can be made available on the (password-protected) conference web page after you've all gone home.

The Avervision document camera is a sort of cool overhead projector. It will display any printed document, photo, slides, X-ray film or 3D object straight through the projector, so basically you can dissect a frog live on the wall. There is a Victorian microscope with an attachment that allows it to be connected to the Avervision, so biological people can project the microworld on the big screen. Although we have a table with a white square painted on it, non-electronic talks are probably better on white pieces of paper rather than on transparencies..

12 EXCURSIONS AND ACTIVITIES

The various excursions and activities are divided into categories according to the physical effort involved. As there will be around 40 people at the conference, it is envisaged that each day the group will split into two or more subgroups, with the hot young muscular virile people doing the strenuous excursions, and the lazy, old and unfit doing more relaxed activities. Although we have incorporated suggested activities into the programme above, everyone is welcome to consider the following list and also to consult the various guidebooks in the TTI library in order to suggest alternative activities.

12.1 Very strenuous activities

- Climb the peak of Pizzo d'Uccello. Requires early start with no other activities (e.g. day before conference). See www.tcm.phy.cam.ac.uk/~mdt26/tti2/photos/pizzo_ducello.jpg. Enough said. They don't call it the 'Matterhorn of the Apuan Alps' for nothing.
- The ascent of Monte Procinto. This is a huge cylindrical rock tower with a belt of trees around its middle from which rise 500-foot walls, overhanging on every side. Michelangelo had the idea of carving it into a gigantic sculpture along the lines of Mount Rushmore but never got round to it. You can see the mountain here: www.vallico.net/procinto.jpg. Yes - the walls are more or less vertical, but there is a *via ferrata* to clip yourself onto. Instruction, assistance, and the

necessary equipment can usually be supplied - but we only have about eleven harnesses so bring your own if you have one!

- Reach the high peak of Pania della Croce from Piglionico (described as ‘The finest peak in the whole of Italy’ in *Below the Snow Line* - one of the 19th century books in the TTI Antiquarian Library). Also features in Dante’s *Divine Comedy*. This defeated some of TTI finest mountaineers for several years before they finally succeeded in 2007 (note - it isn’t that hard if you move quickly).
- Find the spectacular natural rock bridge of Monte Forato (under which someone once flew a bi-plane). Start from Fornovolasco (lots of up) or from Matanna (much easier) or even have two groups that meet in the middle and exchange car keys. New for 2009: there is a fun via ferrata traverse on the way to the arch from Matanna, and we will do a new route via Foce di Valli.
- Find the Neanderthal cave (Grotte all’Onda) down the slope from the balloon station near Matanna. *”This vast grotto stretches 40 x 60 meters and it originally hosted numerous internal tunnels, which are obstructed today. Its enormous cavity offers important evidence that suggests the frequency with which people entered the grotto, from pre-historical times to more recent periods. The first people to use the cave were Neanderthals; they hunted throughout the surrounding area and probably used it to hoard their tools and weapons, together with the bones of the animals they cooked. Hunters from the Superior Palaeolithic period (Homo Sapiens) lived in the more external part of the grotto where they set up a giant hearth. Later, Neolithic farmers and shepherds planted their huts in the shelter of the grotto’s vast vault, carrying out their daily activities there during many seasons. This cave was also used during the Neolithic period (the Bronze Age), during which new models were developed for decorating ceramic. During this period, new raw materials, imported from distant locations, were adopted to make special equipment. From the post-Bronze Age until recent times, the grotto was not continuously frequented.”*
- The new Geoscopio web site (www.vallico.net/tti/tti_mountaineering.html) shows precise locations of all of the thousands of caves in Tuscany (even the crap ones) together with a brief technical description and a plan of the cave. Interesting little expeditions may be made that have the aim of finding the entrance to particular caves, as well as exploring them. This is of course the most fun that a boy can have. The Apuan Alps have more caves than you can possibly imagine, so this will still be a viable activity in 2050. In particular, ask Mike about the untried Campolemisi, Fabbriche di Vallico, Motrone, and Antro della Paura expeditions.
- Explore the canyon of the Turrite di San Rocco river. This starts from the fork in the river upstream from Fabbriche di Vallico before you get to Gragliana. Take the left-hand fork. The aim is to go all the way through it to take coffee at the cafe near the Chiesa di San Rocco in Turrite. Be prepared to get wet - you basically can’t avoid it. There are various natural swimming pools in there. Once reaching the village where the cafe is (there is also a children’s playground and a nice river) you will have to bribe a local to give your driver a lift back via Focchia to your van. Or perhaps all your drivers drove a convoy out there beforehand, left most of the vehicles, and returned to the start of the canyon in a single car - use your initiative here.
- Morning workout. Run from the Institute each morning at 6am to the spectacular summit of Monte Palodina in order to tone up your thigh muscles and pep yourself up in preparation for the morning’s talks. Mad people only.
- Complete the Cinque Terre coastal walk, a four-hour excursion through some of Italy’s most spectacular scenery, or a similar walk near the famous seaside haven of Portofino.
- *Orrido di Botri* canyon walk. The Orrido is a giant canyon created by the Pelago river in the Apennines (about an hour’s drive from the Institute) with deep steep walls as high as 200 metres and in some places only a few metres apart. This is a geologists’ and naturalists’ paradise. It can only be visited with helmets and suitable clothing you don’t mind getting wet. There are some nice long walks in the country above the canyon (watch out for marmites and Royal Eagles - this is one of your best chances to contribute to the TTI Wildlife Photography expedition).
- There are of course any number of spectacular high mountain expeditions in the Apuan Alps and the Institute has a library of guidebooks which you can browse through. Let me know if you want

to try anything else (that will fit in the clearly limited amount of time). There is also the TTI Antiquarian library (Mountaineering section) to inspire you.

12.2 Quite strenuous activities

- Go to Alto Matanna at the end of the Turrtecava valley and visit the beautiful nineteenth-century hunting lodge that was once the destination for travellers in Rosetta the Balloon on her aerostatic cableway. See the old balloon station at Foce del Pallone and the extraordinary view. On clear days you can see Elba - 100 miles to the South - and sometimes the even more distant Corsica and the French Alps. Come back over the top of Monte Matanna and descend back to the lodge. Take one of the Institute's antique telescopes with you.
- From the Matanna hotel, climb up to the cross on the adjacent ridge for a spectacular view of Monte Procinto, Stazzema and the Apuan Alps. From there you can climb Monte Matanna the other way around, or visit the donkey and his little horse friends who live on the top of Monte Nona. Or you could go on a longer walk below the Giant West Wall of Nona, threading past Monte Procinto, and round the back of Monte Nona which will take several hours. Finish up the day with a fabulous dinner in the Matanna hotel.
- Take part in the latest expedition to the ancient cave known as the *Tana di Cascaltendine* which is the subject of Pietro Magri's 1880 book *An expedition to Mount Gragno and the Cave of Cascaltendine* as translated by Mike and available on the TTI web site (click the Local History Projects link). The 2007 summer school crew were able to photograph the result of the following quote : *'Before coming down from the cavern we used a chisel to inscribe our initials and the year 1880 on both walls of the passage near the entrance.'* This was done in the "Palace of Ismeno" which was the name Magri's group gave to an extensive cave whose entrance is a 6 foot hole about forty feet up a cliff - the full story is on the News from the Towler Institute blog. It is also known that the cave continues for a kilometre beyond where we have penetrated before and this remains to be explored (note that in summer 2007, Mike and Evans went up the big wall in the final chamber with the dangling rope - a place many TTI visitors have visited before - with somewhat amusing consequences - see the blog story 'Bronze Hermaphrodites and the Fat Boy Filter'). Expedition to be followed by cold beers and refreshments in the lovely village of Cardoso, or a circuit of Monte Penna hunting for the lost Cave of the Fairies..
- Visit the Selva del Buffardello adventure park:

www.selvadelbuffardello.it/index.php?lang=eng

I quote from their web site: *"Among the centuries-old fir trees some acrobatic forest paths, open to everybody, have been created and their aim is to show the wood from a different and adventurous point of view: hanging in the air. It is a challenge for children, youth and adults, who can test their ability with suspension bridges, swinging beams, vertical nets, ropes and obstacles, finding again their lost adventurous spirit. The Adventure Park 'Selva del Buffardello' in San Romano in Garfagnana (locality Pra' di Lago) is a real novelty in the Appennino Tosco Emiliano. An old wood of two hectares and a half in the heart of Garfagnana, near the natural 'Parco dell'Orecchiella', with a wonderful view on the Alpi Apuane and on the Fortezza delle Verrucole (old castle). The park entrance is free if you don't practise in the adventure paths."* We have never tried this, but it looks like great fun.

- TTI management has discovered that there is a secret underground tunnel in Vallico which starts from the Doctor's House next door to the Institute (a former barracks) and which goes up to the Rocchetta above the village (the site of an old castle on the summit of a little hill, where we now pitch the Bedouin Tent). This was used in mediaeval times for escape from the frequent warfare so common in these parts. The supposed entrance to the tunnel was bricked up (we think) in the 1930s - there are a couple of elderly men in the village who vaguely remember it. This summer we hope to unblock the entrance and explore. We also wish to find the upper entrance, so if you know anyone who has a ground-penetrating radar set we can borrow, let us know. This will probably be one of the next thrilling tales in 'News from the Towler Institute'.

- Explore the Vallico Sotto mule trail and the spectacular forgotten waterfall of Cascata Pendolina - one of the highest in Italy. Vallico was only connected by road to the outside world in the 1960s - before then people went up and down the *mule trail*. This has now been forgotten and is a little overgrown (though less so following TTI clearing activities) but is still very beautiful. Once we reach the bottom of the valley we will head over the river to the site of the Cascata Pendolina where we will take lunch. On the way back the bravest people will try to ascend the *Canyon of the Pili* carved by the Rio Selvano (you will get wet!). EDIT: and they will fail - I have recently discovered the only way you can feasibly do this is to *descend* from the top. Apparently this canyon is quite famous - the Apians group from Castelnuovo organize tours through it. One of these days I will have to attach myself to one of these expeditions to learn how to do it. Apparently there are 12 major waterfalls to descend - photos and rough maps are linked from the Mountaineering page of the web site.
- Explore *Buca della Freddana* cave near the mule trail from Vallico Sopra to San Luigi. This was (re-)discovered by Mike in Easter 2007 following conflicting and confusing advice from several local old ladies who remembered its existence from 40 years ago. He has also found the upper entrance of the same cave on the summit of Monte Penna - the two are apparently connected by a 1 kilometre passage. The old ladies have advised us not to go inside because of the evil monsters and dark pits that lurk within, but then again, they always say that. Dare you explore?
- Five a side-football (a new fenced pitch was constructed in Vallico a couple of years ago) or regular football (on the local full-sized pitch).
- Rock climbing or low-level bouldering - the Institute should have some ropes and climbing equipment. I've read that there is good climbing near the Trombacco dam in the next door Fornovalasco valley - ask MDT for more details. Don't forget to bring climbing boots and a harness that fits if you want to do this seriously (we have a rope you can borrow).
- Pietro Magri in his 1880 book mentioned above states that there are two other caves in Monte Gragno besides the Tana di Cascaltendine. Today no-one seems to know where they are. Having found the Buca della Freddana, Mike has narrowed down the lost "Cave of the Fairies" to a relatively small area. Can you find it?
- Traverse from Santa Luigi via Monte Palodina and the cliffs of Monte Gragno past the giant karst depression of Pian di Lago to the spectacular Rocca Estense fortress of Trassilico. Come back along the road past La Fornace.
- Explore the *Tana che urla* (the Cave that Screams!) - first explored and scientifically described by Vallisneri in 1726 - off the footpath to Foce di Petrosciano from Fornovalasco. This isn't a tourist cave suitable for your mum - so bring some appropriate clothes and torches. By the summer the Institute should have some proper speleological equipment to hand round. If you can read Italian, have a look at www.buffardello.it/attivita/pubblicazioni/di_alcune_grotte.pdf.
- Go on a beautiful walk over the highest stone railway bridge in Europe to the church in Sambuca.
- Go wild boar hunting.
- Learn to play local sport *palla elastica* (elastic ball) with the village youths.
- Use TTI's two inflatable boats to play on the Turrtecava lake - accompanying picnic recommended. Have races. Try to find the Buca del Lago della Turrtecava (as you sail towards the dam, it is on the left just after the exit of the second road tunnel).
- Go kayaking on the Turrtecava. Bring your own canoe.
- Explore the ancient *Vasaio di Motrone* cave in the nearby village of Motrone (see www.apuane2007.it/italiano/vasaio/zona.vasaio.php).

12.3 Relaxed activities

- Visit the Pinocchio park, the Garzoni gardens, and the Collodi butterfly house in Collodi. See www.pinocchio.it/park.htm. From the website: *“Inaugurated in 1956, the Pinocchio Park is no ordinary theme park, but rather a precious masterpiece created by artists of great character working together. The literary itinerary, marked out by mosaics, buildings and sculptures set amidst the greenery, emerges from an inspired combination of art and nature. The path is winding, and the dense vegetation means that every stage on the route comes as an unexpected surprise, with the very plants and trees contributing to create the atmosphere and the episodes in the story of the Adventures of Pinocchio. The Park itself is the site of constantly renewed cultural activities that are always mindful of its roots: exhibitions of art and illustrations inspired by childrens literature and the Story of Pinocchio, puppet-making workshops, puppet and marionette shows and minstrels enliven the visit to the Park, depending on the season. ”. For the gardens: “The historic Garzoni Garden, one of the most beautiful in Italy, represents a felicitous synthesis between Renaissance geometry and the spectacular quality of the nascent Baroque. The garden is a work of art of rare equilibrium, where the greenery, the flights of steps the water plays and statues form a truly unique ensemble. It is an absolutely unforgettable experience to lose oneself amidst the wonders of this fantastic place: grottoes, theatres carved out of box hedges, statues representing mythological creatures, satyrs, female figures, greenhouses with peacocks, forests of bamboo. An ancient, and somewhat arch tradition considers the visit to be propitious for lovers, and not only on account of the leafy shade and the arbours that offer secluded spots for tender caresses, but also of the maze, a symbolic allusion to the path to follow together throughout life. As soon as we enter the garden we come upon delightful parterres, statues and two large circular pools. Proceeding we then reach two magnificent double ramps of steps featuring a complex hydraulic system that supplies the water plays. These steps lead to the three upper terraces. Beyond is the impressive water staircase, flanked by two female statues representing the eternal rivals Lucca and Florence. At the very top is the statue of Fame blowing into a shell, emerging from which a jet of water traces out a lofty arc. Leading off the main route through the garden are numerous side paths and avenues where we can discover its marvels among the fragrances of the different plants, the plays of light and shade of the vegetation, the intrigue of the mazes and the enchantment of the sculptures. The garden has recently been restored.”*
- The Opera Barga festival is usually on at the same time as the conference (25th July-8th August in 2009). Ask Mike in advance for tickets and reservations.
- Look in the latest issue of Lucca “Grapevine” magazine in English for local cultural activities and concerts etc..
- Play with the Institute’s Victorian Scientific Instrument Collection.
- Spend the afternoon bathing in the outdoor hot pool at the ancient thermal baths of Bagni di Lucca (one of the most fashionable spots in Europe in Lord Byron’s time - the Switzerland of Tuscany!). Followed by shopping, sightseeing and coffee in the town centre.
- Samantha has two other favourite open-air pools at Galliciano and Barga. These are like little beach resorts where one lazes about on deckchairs and has the occasional dip.
- Watch the night sky through the Institute’s astronomical telescope.
- Visit the ancient city of Barga (www.barganews.com) for an afternoon’s relaxed sightseeing, shopping and culture.
- Visit the beautiful city of Lucca.
- Visit Castelnuovo di Garfagnana, where you can find Andrea’s (the ‘Indiana Jones of the Garfagnana’) famous Osteria, where all day you can sample fabulous local wines, cheeses and snacks.
- Follow in the footsteps of Michaelangelo, and visit some of the Apuan Alps famous marble quarries.
- Day trip to Florence.

- Drive to the next valley along from ours over a spectacular high mountain road where the eagles live. Visit the Grotta del Vento - the Cave of the Winds (www.grottadelvento.com). This is the most famous cave system in Tuscany and the visitor will enjoy a spectacular and bizarre landscape of caverns and lakes. Take a pullover as the temperature is a reliable 10 degrees the whole year round. Then head down the valley to visit the *Eremo di Calomini* - an ancient monastery built into a high steep cliff.
- Table football and drinking in Fabbriche di Vallico.
- Horse riding at La Fornace.
- Various mild short walks around the Institute.
- Digging the Institute garden and doing little DIY things like restoring the church or clearing paths (I say this merely in hope..).

12.4 Very relaxed activities

- TTI now has a high-definition video camera. Make a film of life at one of the world's best conferences.
- Budding archaeologists may use the TTI metal detector - bought following last year's spooky event when Evans and Mike were digging a hole in the ground for the satellite dish (I'm really not making this up): MIKE: Hey Evans, watch out for crucifixes when you're digging that hole. This used to be a monastery you know. EVANS (REACHING INTO THE HOLE) What, like this one? (HOLDS UP A THOUSAND YEAR OLD BRONZE CRUCIFIX FROM FIVE FEET DOWN).
- Spend all day in the TTI garden relaxing in one of the Institute's three hammocks, drinking wine, snoozing or reading one of the books from the TTI library.
- The Institute has a variety of board games, jigsaws, and similar entertainments together with a number of Victorian books with titles like 'What To Do On Cold Winter Evenings Given That We Haven't Invented Television Yet'.
- Debate physics with the help of the Institute blackboards.
- Listen to one of Mike's tedious lectures inspired by the contents of the TTI Antiquarian Library such as *Richard Burton and the Source of the Nile* (Burton the Victorian explorer and polymath, not the one out of *Where Eagles Dare*..) or *Up The Orinoco with Alexander von Humboldt*.
- Spa treatments in the Bagni di Lucca "Thermal resort".
- Mike is translating some chapters of a book on the history of Vallico Sotto. If he's finished it by the time you visit, then walk around the village looking at the buildings and places it describes.
- MDT has taken to writing stories about events at the Institute and publishing them on his blog at the local Barga News website. See www.barganews.com and the "News from the Towler Institute" blog (or go to the TTI web site www.vallico.net/tti/tti.html and click on the relevant link in the left-hand column). So far these are mainly about cave explorations and similar adventures. However, Mike doesn't have a monopoly on this. If you wish to contribute your literary efforts then please send your stories about your adventures in Italy to him, and they will be published on the blog.

12.5 General

- The Institute has a wildlife photography notice board. Prizes for the best entries, particularly if you can take a picture of one of the eagles that regular soar above Vallico or of the elusive *marmite*.
- The Towler Institute Exploration Society also has a photographic competition running - see the web site for details.

- Revitalize the economy of Vallico Sotto. It's barely 40 years since 450 people lived here. Now less than 100 do so. Just because modern lazy teenagers want to be fashion models smoking drugs in Milan rather than having a nice healthy outdoor life, the population of rural Italy has been denuded. Let's bring back the time when all the mountain terraces were in production, packs of nice mules helped carry things, teams of volunteers kept paths and bridges open, and everyone knew how to bake chestnut cakes. All serious suggestions gratefully received.

13 FOOD

In general breakfast will be taken in the Institute, and lunch in the little bar in Vallico Sotto run by the lovely Monica.

In the institute some basic food staples will be provided which participants should feel free to fight over but in general you might like to buy your own food in the village shop run by the lovely and friendly Adelina. However sadly you can't because it closed in late 2007 - much to the consternation of all she has now relocated to a big new shop down in the main valley in Pian di Coreglia. To replace her, there are two food shops in Fabbriche di Vallico - five minutes drive downhill, and a giant Leclerc supermarket in Galliciano (twenty-five minutes drive).

To find the Vallico Sotto bar for lunch, go down the tunnel underneath the Doctor's house (the big house opposite the TTI church front door). Then take any path downwards until you get to the Vallico main square - the bar is just underneath that.. You are strongly encouraged to take your lunch here, as normally it doesn't serve food and Monica is doing us a big favour by buying food and preparing it - so we need to make it worth her while . Note you can also get beers and coffees and so on here..

Note that people in local shops - or indeed anywhere round here - tend not to speak English, so learning some basic Italian food words before you come will help : *pane* = bread, *formaggio* = cheese, *prosciutto* = ham, *pomodori*=tomatoes, *birra* = beer, *vino* = wine, *caffè* = coffee, *latte* = milk, *grazie!* = thank you!.

You are of course welcome to make use of the Institute's cooking facilities whenever you want; in fact why not cook a lovely meal demonstrating the delicious cuisine of Kazakhstan, or wherever it is that you come from? There is a big downstairs kitchen in the main building with a total of 10 rings formerly run by a proper cook, and a small upstairs kitchen. The Institute even has its very own *Il Collegio Cookbook* written and published by former owner Leonie Whitton whose recipes you are encouraged to try. There are also two kitchens in the adjacent Doctor's house which will be rented for the duration of the conference, and similar facilities in most of the other houses.

On the first evening a simple buffet dinner will be provided. Later in the week the Institute's 16th Century pizza oven may be pressed into service. The rest of the time we will make use of the excellent local restaurants - these are mostly incredibly cheap. When very large numbers of people are staying at the Institute, people are encouraged to break up into at least two groups, although many of them - especially Da Sandra - are large enough to handle everyone. Unless told otherwise, Mike will simply assume that you will be coming to each evening meal and will make bookings accordingly (generally a few weeks in advance). These bookings can be changed but please give Mike plenty of notice.

Finally, if you are a vegetarian, you need to be aware that the locals will consider you to be certifiably insane and will feel very sorry that you are unable to enjoy their passion for delicious animal products of all kinds - particularly those made from parts of pigs. Don't worry about this. Following almost a decade of TTI activities, they are now used to us bringing strange foreigners to their restaurants and most are now able to supply vegetarian meals of some kind.

A FEW LOCAL RECOMMENDED RESTAURANTS

- Mulino Biologico (3280 707037, Fabbriche di Vallico)
- Da Sandra (0583 761289 on the road between Fabbriche di Vallico and Vallico Sotto).

- Il Canapale (0583 761829, Vallico Sopra)
- Al Laghetto (0583 75798, near the lake at the entrance to the Turrtecava valley)
- La Rondine (0583 761751 Fabbriche di Vallico, open Fri evening, plus all day Sat/Sun)
- Alto Matanna (0584 776005, Matanna)
- Ristorante Rita e Rinaldo (0583 357728, Focchia)

RESTAURANTS SLIGHTLY FURTHER AFIELD

- Circolo dei Forestieri, Bagni di Lucca
- Antica Trattoria dell'Eremita, Vergemoli
- Il Garfagnino, on the main road near Turrtecava.
- Quadrifoglio, on the main road near Calavorno.
- LOTS MORE - ASK

SPECIAL RESTAURANTS

- La Buca di Sant'Antonio, Lucca
- La Mora, Ponte a Moriano
- Butterfly, Lucca

See also the TTI Restaurant Guide page on the website.

14 CLEANING ROTA

Guests who have the misfortune to be members of the Cambridge University TCM Group and under the age of 40 are normally press-ganged into trying to keep the Institute clean:

Mike Towler - upstairs kitchen and corridor, church
 Bartomeu Monserrat-Sanchez - back garden, church
 Gareth Conduit - upstairs bathroom
 Jonathan Lloyd-Williams - middle corridor and bathroom, front porch
 Edgar Engel - downstairs living room , corridor and pantry, front garden
 Pascal Bugnion - downstairs kitchen
 Peter Townsend - downstairs kitchen

Everyone else please try not to create too much mess for them.

15 CINEMA VALLICO

The requirements of modern science presentations means the Institute church is also the only cinema in the whole of the Apuan Alps - a fact that local people very much enjoy (since the opening presentation of *Cinema Paradiso* in August 2005). During the conference you are welcome to use the projectors and it is expected that movies will be shown on some evenings. The Institute has an extensive DVD library which you are welcome to browse. Feel free also to bring your own movies that you think we might enjoy.

16 NEWS FROM THE TOWLER INSTITUTE

MDT occasionally writes stories about events at the Institute and publishes them on his blog at the local Barga News website. See www.barganews.com and the “News from the Towler Institute” blog (or go to the TTI web site www.vallico.net/tti/tti.html and click on the relevant link in the left-hand column). So far these are mainly about cave explorations and similar adventures. However, Mike doesn’t have a monopoly on this. If you wish to contribute your literary efforts then please send your stories about your adventures in Italy to him, and they will be published on the blog.

17 FOOTBALL MATCH: VALLICO SOTTO CONTRO IL MONDO

The thrusting young lads of Vallico Sotto have challenged the Rest of the World - i.e. you - to a game of 5-a-side football on the village pitch. This tradition - which we began a few years ago - attracts a large crowd and we always get absolutely caned (even when I have had Brazilians and Spanish people available). Can a small mountain village with less than a hundred inhabitants continue to defy the other 6 billion of us? If you think you can stop them, please volunteer.

VOLUNTEERS REQUIRED

Lucas Wagner

Peter Townsend

Tack Uyeda

Pierre-Francois Loos

18 SUMMER SCHOOL

Note that the conference will be followed by a QMC Summer School the following week, taught by Mike Towler, Neil Drummond, and Pablo López Ríos assisted by Martin Krupicka. Schedule available on the web site. Volunteers to help are absolutely welcome - particularly if you can drive.

19 MUSIC

Participants with musical talents are encouraged to demonstrate them in the evenings. We have an acoustic guitar, a Line 6 Variax 500 electric guitar, a Line 6 guitar amplifier (with built-in effects), a top-of-the-range (for 1995, and still very good) Technics keyboard with a decent set of drum accompaniments and excellent piano sound, an electric violin, and 2 microphones. We also have an antique 17th-century violin (broken). There is a Yamaha Stagepas-300 PA system with built-in mixer into which anything electronic in need of amplification may be plugged. Note the Variax 500 is a *modelling guitar* (i.e. internal electronics process the sound from individual strings to supposedly model or replicate the sound of specific guitars and other instruments.)

On payment of a suitable fee (such as a cigarette, which he only smokes during TTI meetings because of the stress), Mr. Mike Towler can sometimes be persuaded to attempt poor-quality Jerry Lee Lewis impersonations on the piano, and Mr. Pablo López Ríos - who is actually a member of a proper band in Cambridge that plays in front of real people for money - is always happy to strum away in a variety of different styles (or he would be if he was actually coming to the conference this year). Mr. Neil Drummond is believed to be able to play the maracas, but we don’t have any.

Note as with all musical performances, practice beforehand is always strongly recommended. Feel free to organize this.. (MDT knows various tunes that could do with some decent backing vocals.).

20 HEALTH AND SAFETY

We should all recognise that climbing, mountaineering and caving are activities with a danger of personal injury or death. Participants in these activities during their stay at TTI are asked to be aware of and accept

these risks and be responsible for their own actions.

The nearest Accident and Emergency Department is 25 minutes away in Barga Hospital (car drivers should satisfy themselves as to its location on Google Maps) - other hospitals are in Lucca (50 minutes) and Castelnuovo di Garfagnana (45 minutes). The Italian emergency telephone number is 112.

Vallico Sotto is a mediaeval village built a thousand years ago on a steep slope with many steps, and naturally there no facilities whatsoever for the disabled; furthermore it seems that the builders of long ago have intentionally set traps designed to kill or injure you. However don't let this put you off; wheelchairs and so on can be manhandled up the hill with you in it if required - think of it as a challenge.

TTI is a smoking venue and visitors may smoke as much as they like (ashtrays will be provided).

21 APPENDIX 1 : Talk abstracts

Some people like to provide abstracts for their talks. The ones I have received are gathered here.

Pascal Bugnion

"Spins, superfluidity, and ultracold atomic gases"

Recent advances [1] allow experimentalists to confine and address individual ultracold atoms in a harmonic trap. We use full configuration interaction and quantum Monte Carlo to demonstrate how this unprecedented level of control can be used to study inhomogeneous pairing in superfluids [2] and the mechanisms behind the emergence of magnetism [3].

[1] F. Serwane et al. Science 332, 336 (2011)

[3] P.O. Bugnion, J. A. Lofthouse and G. Conduit, (Accepted in Phys. Rev. Lett.) arXiv 1305.3717

[3] P.O. Bugnion and G. Conduit, Phys. Rev. A 060502(R) (2013)

Gareth Conduit

"Concurrent materials design"

We have developed a new computational tool to model, characterize, and discover alloys that simultaneously fulfill up to ten different physical criteria. The concurrent materials design paradigm would mean that engineers will no longer have to compromise objects and products around non-ideal and pre-existing materials, but can optimize materials for a specific purpose, bringing materials into the heart of the design process.

Using the tool we have discovered three new Ni-based polycrystalline alloys and two Mo-based forging alloys, principally for use in gas turbine engines. Experimental testing has demonstrated that the proposed alloys fulfill the computational predictions to match or exceed the properties of commercially available alloys, so they are now being conformance tested by Rolls Royce plc.

Patent GB1302743.8 (2013)

Patent GB1307533.8 (2013)

Patent GB1307535.3 (2013)

Mike Gillan

"Quantum Monte Carlo benchmarks for weak non-covalent interactions"

Without hydrogen bonding, life would cease, the oceans would boil, and all wooden structures would collapse. Weak non-covalent interactions like hydrogen bonding and dispersion are indeed crucial for the properties of all kinds of molecular materials! Density functional theory has great difficulty in describing these interactions problems with water have been well publicized, though this is only one of many examples but there is now abundant evidence that diffusion Monte Carlo is very accurate for non-covalent interactions [1]. An international INCITE project involving several participants in the present workshop has been set up to use DMC to provide energy benchmarks for a range of molecular materials. I will introduce this project, stressing its aim to use DMC benchmarks to help test and improve dispersion-inclusive DFT approximations, force fields and emerging electronic-structure methods. I will give some illustrations from recent work [2] in which DMC benchmarks for water nano-droplets, ice structures and liquid water in periodic boundary conditions have been used to analyze the errors of chosen DFT approximations. This work shows that DFT problems with water are not due only to deficiencies in describing dispersion.

If time permits, I will also outline a completely different electronic-structure approach to the energetics of molecular systems, based on an 'embedded' many-body expansion implemented using the second-order Moeller-Plesset and coupled-cluster approximations. I will show that this approach gives an extremely accurate account of the absolute and relative energies of different ice structures [3], and I will suggest that comparisons with DMC benchmarks for a variety of molecular systems could be a very fruitful way of exploring the capabilities of embedding techniques.

[1] I. G. Gurtubay and R. J. Needs, *J. Chem. Phys.* 127, 124306 (2007); B. Santra, A. Michaelides, M. Fuchs, A. Tkatchenko, C. Filippi, and M. Scheffler, *J. Chem. Phys.* 129, 194111 (2008); B. Santra, J. Klime, D. Alfe, A. Tkatchenko, B. Slater, A. Michaelides, R. Car, and M. Scheffler, *Phys. Rev. Lett.* 107, 185701 (2011); M. J. Gillan, F. R. Manby, M. D. Towler, and D. Alfe, *J. Chem. Phys.*, 136, 244105 (2012).

[2] D. Alfe, A. P. Bartok, G. Csanyi, and M. J. Gillan, *J. Chem. Phys.* 138, 221102 (2013).

[3] M. J. Gillan, D. Alfe, P. J. Bygrave, C. R. Taylor, and F. R. Manby, arXiv:1307.3767 (2013).

Natalia Matveeva

"Localization of an impurity in a bilayer system of dipoles"

We consider a bilayer geometry where a single impurity moves in a two-dimensional plane and is coupled, via dipolar interactions, to a two-dimensional system of fermions residing in the second layer. Dipoles in both layers point in the same direction oriented by an external field perpendicular to the plane of motion. We use quantum Monte Carlo methods to

calculate the binding energy and the effective mass of the impurity at zero temperature as a function of the distance between layers and of the intralayer interaction strength. In the regime where the fermionic dipoles form a Wigner crystal, the physics of the impurity can be described in terms of a polaron coupled to the bath of lattice phonons. By reducing the distance between layers the effective mass of this polaron exhibits a crossover from a free-moving to a localized regime with a localization length significantly smaller than the lattice spacing.

Have fun in Vallico Sotto!