

Quantum Monte Carlo in the Apuan Alps II

International Workshop
Sat 22nd July - Sat 29th July 2006
The Towler Institute, Vallico Sotto, Tuscany

www.tcm.phy.cam.ac.uk/~mdt26/tti/tti.html

July 21, 2006

This is the final programme for the second international quantum Monte Carlo workshop to be held at the Towler Institute. As with all such events at the Institute, *Quantum Monte Carlo in the Apuan Alps II* is designed as a holistic alternative to the regular 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 will be organized in the afternoons, and it is hoped that by following this strict regime, together with breathing clean mountain air and by preparing and sampling fine Tuscan cuisine, the participant will be able to return home mentally and physically refreshed as well as better informed. This is especially likely to be the case if, as is all too common in our profession, the participant normally spends all of his or her time shut up in a dark office with a computer. We hope you have fun at the Towler Institute!

1 LIST OF PARTICIPANTS

Ali Alavi	Cambridge University (Chem.)	asa10 at cam.ac.uk
Alan Aspuru-Guzik	University of California, Berkeley	CANCELLED
Alexander Badinski	Cambridge University	ab582 at cam.ac.uk
Dario Bressanini	Università dell'Insubria	dario.bressanini at uninsubria.it
Neil Drummond	Cambridge University	ndd21 at cam.ac.uk
Matthew Foulkes	Imperial College, London	m.foulkes at ic.ac.uk
Idoia Garcia de Gurtubay	Cambridge University	ig243 at cam.ac.uk
Ainsley Gibson	Howard University	ainsley.gibson at gmail.com
Richard Hennig	Ohio State University	hennig.4 at osu.edu
Nick Hine	Imperial College, London	nicholas.hine at imperial.ac.uk
Pablo Lopez Rios	Cambridge University	pl275 at cam.ac.uk
Andrea Ma	Cambridge University	am570 at cam.ac.uk
Ryo Maezono	NIMS, Tsukuba, Japan	maezono.ryo at nims.go.jp
Lubos Mitas	North Carolina State University	lmitas at unity.ncsu.edu
Richard Needs	Cambridge University	rn11 at cam.ac.uk
Zoltan Radnai	Cambridge University	zr205 at cam.ac.uk
Ian Snook	RMIT University, Melbourne	ian.snook at rmit.edu.au
Graham Spink	Cambridge University	ggs24 at cam.ac.uk
Mike Towler	Cambridge University	mdt26 at cam.ac.uk
John Trail	Cambridge University	jrt32 at cam.ac.uk
Paolo Umari	Massachusetts Institute of Technology	CANCELLED

Samantha Keil and Saska Towler
Marie Snook
Dori Aspuru-Takata CANCELLED
Sanam Alavi CANCELLED
Stacy Hennig

2 FLIGHTS AND TRANSPORT

This section gives details on how to get to the Institute for people flying into Galileo Galilei Airport, Pisa. Further details about transport, including how to drive to the Institute, are given on the TTI web site.

The participants will mainly arrive in two groups:

The Cambridge and Imperial groups will arrive on Friday 19th July (Flight 584 at 06:30 from Stansted arriving in Pisa at 09:45). From Pisa airport they will drive the hired transport (one large minibus and two cars) to the TTI. Designated drivers : Alexander Badinski, Idoia Garcia de Gurtubay, Pablo Lopez Rios.

Everyone else should aim to arrive at Pisa airport on Saturday 22nd July. 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, but if you really need to arrive early this can be arranged - contact Mike. Late departures could be problematic however because of the summer school taking place immediately after the workshop - again, let Mike know if this affects you.

How to get to the TTI from Pisa airport on Saturday 22nd July:

Go to Pisa Centrale train station - either by taxi in 5 minutes from the airport or by a short train ride from Pisa Aeroporto station (which you get to by walking out of the left-hand side of the airport). You then want to get a train to Barga-Galliciano. This is north of the city of Lucca 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" or "Minucciano" though I can't guarantee this is true for all of them. Don't forget that in Italy you need to validate your train ticket by getting it stamped in the yellow machines on the platform or you may have to pay a fine. Other than that, Italian trains are absurdly cheap by international standards.

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 (driving either a minibus or a maroon Fiat Multipla). If no-one is there you can wait in the excellent station café until he arrives - do call if you have to wait more than five or ten minutes. Clearly it would be helpful if participants could state in advance the time of the train on which they intend to arrive. The timetable is linked from the TTI web site - don't worry about the fact that this is the German Railways timetable - it's just better than the Italian equivalent. Currently the timetable suggests that train arrivals at Barga from the direction of Lucca are at 6.54 7.37 9.13 12.13 14.12 14.50 16.28 17.40 18.57 20.15 21.34 and 22.20 (corresponding to departures from Lucca at 6.12 8.25 11.30 13.25 14.10 15.47 16.58 18.17 19.36 20.46 21.40). Note that the last train from Pisa appears to be at 20:50 .

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 : taxibarga@libero.it Tel. 340 1669279 or 348 8106112). If you are a non-Italian speaker who hasn't pre-booked and need to talk to the guy on the phone you will find he doesn't speak English so just say (phonetic) "Taxi a Vallico Sotto da la stazioni di Barga? Inglayzi. Non parlo italiano." or similar down a phone at him - the trip should cost 30 Euro.

In case of problems contact Mike on his mobile phone - 3478077359. Additional assistance is available from Samantha Keil on 3478077418. The TTI has a direct phone line (0583 761706) but this should be used as a last resort as people generally need this for internet use.

3 TRAVEL SPECIFICS

Here are the final travel arrangements

FRIDAY (TRANSPORT TO TTI IN RENTED VEHICLES)

Alexander Badinski

Neil Drummond

Matthew Foulkes

Idoia Garcia de Gurtubay

Nick Hine

Pablo Lopez Rios

Andrea Ma

Zoltan Radnai

Graham Spink

John Trail

Lubos Mitas ARRIVE Pisa 5pm, TTI PICKUP FROM BARGA-GALLICANO 18.57

SATURDAY

Ian Snook, Marie Snook ARRIVE BARGA_GALLICANO 21.34, TTI PICKUP

Ryo Maezono TTI PICK UP FROM BARGA-GALLICANO 14.50

Richard Hennig, Stacy Hennig TTI PICK UP FROM BARGA-GALLICANO 14.50

Dario Bressanini ARRIVE OWN CAR (POSSIBLY SUNDAY)

SUNDAY

Ainsley Gibson ARRIVE PISA 9.35, ARRIVE BARGA-GALLICANO 14.50 (TTI PICKUP)

Ali Alavi ARRIVE BARGA-GALLICANO 18.57, TAXI TO TTI (MDT BOOKED)

TUESDAY

Richard Needs ARRIVE PISA 11.45, ARRIVE BARGA 14.50, TAXI TO TTI (MDT BOOKED)

LAST MINUTE CANCELLATIONS

Alan Aspuru-Guzik, Dori Aspuru-Takata

Sanam Alavi

Paolo Umari

4 THINGS TO BRING WITH YOU

Whatever you like, plus :

- The overheads for your talk, if you're giving one - see later section for supported formats.
- Your laptop, if required - see note in next section.
- Summer hiking gear such as boots, socks, mini-rucsacs 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.
- A towel
- Some Euros for spending in restaurants and shops. 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 right as you emerge into the arrivals hall.
- People who intend to visit caves should bring some clothes that you don't mind getting wet and a torch. The clothes can also be used in the Orrido di Botri canyon walk.
- Sunscreen

In the traditions of the first workshop, you might also optionally like to bring

- A nice bottle of wine
- An interesting thing

Remember that squishy luggage is easier to fit into multiply occupied cars than giant hard-shelled suitcases.

5 TTI TECHNICAL EQUIPMENT

There are two Sony Vaio and four Acer Ferrari 4005 laptops in the Institute available for public use (plus Mike's personal laptop, which can be borrowed for short periods) all in dual-boot configurations running Suse Linux 9.3/10.0 and Windows XP.

All connections are made through a WiFi wireless network (802.11b or 802.11g). If you wish to bring your own laptop then it therefore needs to be wireless-enabled if you wish to log into the network. Three spare wireless network cards that you can plug into your laptop PC card slot are available - but note this can be tedious to set up on some machines so clearly it is better to wireless-enable it before you come. 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.

I'm afraid that for the moment the Institute is still on dialup (the wireless network plugs straight into the telephone through a Wiflyer router). Large files should thus be brought with you on your laptop rather than downloaded when you get there. The connection is certainly fast enough for multiple people to do remote logins and terminal-based email. Viewing graphical internet pages is OK when only one person is doing it so try to do this sparingly. Finally, please turn off things like Microsoft's Automatic Update feature - downloading Gb of files to patch all the security holes in your machine while other people are trying to work is not a good idea.

The TTI management is very sorry about the slow connection but would like to stress how difficult it is to get a decent broadband connection in rural Italy. Italian fast connections are almost all ADSL and this is never going to get to such a remote area. It is possible to get satellite equipment but this is currently

beyond our financial means and apparently there is a time delay problem typing on remote computers anyway. We seem to be only a year or two from having appropriate technology to wire the Institute properly with the outside world - such as Wimax or floating giant airships sailing over Europe and so on. In the meantime, all suggestions for improving connectivity will be gratefully received.

Apart from computers and networking devices, we also have the following equipment available for conference participants to use:

- Canon Pixma ip4000 colour inkjet printer (on a wireless print server, so one can print from anywhere in the Institute)
- Hi-Ti Transphotable photo printer 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
- Two memory sticks
- Driver disks for most of the above.
- A supply of writeable CD-Rs, CD-RWs and DVD-Rs.
- the usual stationery and staples etc..

A technical guide to the TTI computer systems will be available in time for the conference. There is also a reasonable selection of scientific reference books, though this needs to be and will be increased..

6 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.

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). If you don't want to bring your laptop, the projector also allows PCMCIA card Mobile disks to be plugged into it. The Institute laptops - equipped with Suse Linux 9.3 and Windows XP - will of course also take CDs and have the usual software such as Acroread and Powerpoint. On balance it is probably best to bring your talk on a CD or email it to Mike beforehand and he will ensure that it is on the relevant machine ready for your talk.

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..

You can of course ignore all the technology and use the blackboard.

7 CONFERENCE SCHEDULE

Here is the schedule for the conference, including a list of talks. This is currently only a rough guide, and the schedule is very malleable. The number of talks per day is deliberately small to allow time for thinking, discussion and deliberation. In principle there will be discussion sessions each evening but last year the participants were so relaxed that these were largely forgotten - time will tell whether participants feel the need to have evening discussions this year. All excursions and activities are, of course, optional. All suggestions gratefully received.

Friday 22nd July

EARLY ARRIVALS

Dinner for 14 booked at Il Canapale in Vallico Sopra.

Saturday 22nd July

ARRIVALS

7.30pm : Welcome buffet dinner and drinks in the Institute garden.

Sunday 23rd July

8.30am : Mike Towler (5 minutes)
- "Welcome to Tuscany"
8.35am : Lubos Mitas (50 minutes)
- "Topology of fermion nodes and pfaffian pairing wavefunctions"
9.30am : Neil Drummond (50 minutes)
- "Ab initio study of positron annihilation in a homogeneous electron gas"
10.30am : Idoia de Gurtubay (30 minutes)
- "QMC dissociation energy of the water dimer: Time-step errors and backflow calculations"

12.30am : CHURCH (your only chance to see the gorgeous Chiesa di San Giacomo in Vallico Sotto - only open during mass on Sundays!).
2.30pm : Trip to Alta Matanna. Three alternative walks available depending on fitness/laziness. See the entire Versilia coast, and even Elba and Corsica from the easily accessible summit of one of the more spectacular mountains in the Apuan Alps. Bring one of the Institute's telescopes. Followed by drinks and dinner in 19th Century hunting lodge. Two of the walks allow you to see the site of the ancient balloon cableway that led up here from the beach (see Local History Projects on the web site).
7pm : Dinner for 20 booked at Matanna
Late : Cinema Vallico

Monday 24th July

8.30am : Richard Hennig (50 minutes)
- "Accuracy of the pseudopotential and fixed-node approximations for first and second-row dimers."
9.30am : Pablo Lopez Rios (50 minutes)
- "Inhomogeneous backflow transformations in quantum Monte Carlo"
10.30am : Zoltan Radnai (50 minutes)
- "Non-collinear spins in QMC: application to spiral spin density

waves"

REGULAR AFTERNOON/EVENING SCHEDULE (Dinner for 20 booked at Da Sandra)

Tuesday 25th July

- 8.30am : Nick Hine (50 minutes)
- "The surface energy of the electron gas: resolving a long-standing contradiction"
- 9.30am : Dario Bressanini (50 minutes)
- "Is QMC delivering its early promises? (with some reflections on nodes and wave functions)"
- 10.30am : Neil Drummond (15 minutes)
- "Some QMC puzzles"

REGULAR AFTERNOON/EVENING SCHEDULE - WITH LONG EXCURSION

Wednesday 26th July

- 8.30am : Matthew Foulkes (50 minutes)
- "Finite-size corrections: structure factor or MPC or both?"
- 9.30am : Ali Alavi (50 minutes)
- "Quantum Monte Carlo based on the idea of sampling graphs"
- 10.30am : Alexander Badinski (50 minutes)
- "Accurate forces from ab initio pseudopotentials within QMC"
- 11.30am : Andrea Ma (30 minutes)
- "The equation of state of diamond"

REGULAR AFTERNOON/EVENING SCHEDULE

Thursday 27th July

- 8.30am : Richard Needs (50 minutes)
- "Where are the atoms?"
- 9.30am : John Trail (50 minutes)
- "QMC: what are the odds of that?"
- 10.30am : Graham Spink (30 minutes)
- "Remaining problems in the homogeneous electron gas"

REGULAR AFTERNOON/EVENING SCHEDULE

Friday 28th July

- 8.30am : Ian Snook (50 minutes)
- "QMC and weak physical interactions"
- 9.30am : Ryo Maezono (50 minutes)
- "The fragment method in QMC"
- 10.30am : Ainsley Gibson (30 minutes)
- "My research"
- 11am : Senior Person (30 minutes)
- "Summary of the conference"
- 11.30am : GENERAL DISCUSSION

REGULAR AFTERNOON/EVENING SCHEDULE

Saturday 29th July

DEPARTURES

The REGULAR AFTERNOON/EVENING SCHEDULE would usually consist of the following:

- * Excursion/activity (see later)
- * Discussion (optional, around 6.30pm)
- * Dinner (see later)
- * Cinema Vallico (see later)

8 EXCURSIONS AND ACTIVITIES

The various excursions and activities are divided into categories according to the physical effort involved. As there will be 25+ people at the conference, it is envisaged that each day the group will split into two, with the hot young muscular virile people doing the strenuous excursions, and the lazy, the corpulent, and those deficient in the requisite number of limbs doing the more relaxed activities. Well-known athletes Mike Towler and Alexander Badinski (especially Alex) will tend to lead the former and Samantha will lead the latter. What to do will be debated in the morning each day - all according to taste! Of course with four vehicles, we can do up to the four activities simultaneously if this is desired.

8.1 Very strenuous activities

- 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).
- Find the spectacular natural rock bridge of Monte Forato (under which someone once flew a bi-plane). This disgracefully eluded the Cambridge student team during last year’s Workshop, probably on account of the city boys’ inept map reading.
- *Orrido di Botri* guided 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. Apparently this is a geologists’ and naturalists’ paradise. It can only be visited on a guided walk with helmets and suitable clothing you don’t mind getting wet. Let Mike know in advance if you want to do this since it needs to be booked.
- Alexander’s morning workout. Run from the Institute with Mr. Badinski 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.
- 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.

8.2 Quite strenuous activities

- Take part in the second 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). This time the aim will be to find and photograph the following things that were missed last summer : The Palace of Ismeno, the Cave of Extreme Fear, the House of Vampires, the Column

of Hercules and the bat. The main aim is 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 whose entrance is a 6 foot hole about thirty feet up a cliff - a picture of which is on the web site. Anyone with rock climbing expertise? Otherwise we will have to somehow get a ladder up there.. To be followed by cold beers and refreshments in the lovely village of Cardoso.

- 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 will take lunch. On the way back the bravest people will try to ascend the *Crystal Canyon* (you will get wet!).
- Five a side-football (a new fenced pitch has been constructed in Vallico since last year) or regular football (on the local full-sized pitch).
- Rock climbing or low-level bouldering - the Institute should have ropes and climbing equipment by the summer.
- Pietro Magri in his 1880 book mentioned above states that there are two other caves in Monte Gragno. Today no-one seems to know where they are. Can you find them? Base camp might be at Santa Luigi ten minutes drive above Vallico Sotto.
- Traverse from Santa Luigi via Mote Palodina and the spectacular cliffs of Monte Gragno past the giant karst depression of Pian di Lago to the spectacular Rocca Estense fortress of Trassilico.
- 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 Fornoalasco. This isn't a tourist cave for wusses - 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/Documenti/alcunegrotte3b.htm.
- Walk over the highest stone railway bridge in Europe to the church in Sambuca.

8.3 Relaxed activities

- Look in the latest issue of "Grapevine" magazine for local cultural activities and concerts etc..
- 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.
- Visit the ancient city of Barga (www.barganews.com) for an afternoon's relaxed sightseeing, shopping and culture.
- Visit the beautiful city of Lucca for the same reason.
- Visit Castelnuovo di Garfagnana.
- Alexander's 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 (I say this merely in hope..).

8.4 Very relaxed activities

- 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 games and jigsaws..
- Debate physics with the help of the Institute blackboards.
- Listen to Mike's lecture "Richard Burton and the Source of the Nile" (Burton the Victorian explorer and polymath, not the one out of *Where Eagles Dare*..) which he didn't have time to give last year, followed by a screening of the "Mountains of the Moon" movie.
- Spa treatments in the Bagni di Lucca "Thermal resort".

8.5 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*. Currently there are seven entries, all taken by enterprising student Andrea Ma.
- The Towler Institute Exploration Society also has a photographic competition running - see the web site for details.

9 DINNER

In general breakfast and lunch will be taken in the Institute. Some basic food staples will be provided which participants should feel free to pillage, but in general you might like to buy your own food in the village shop. The lovely and friendly Adelina will be happy to help you (she doesn't 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!). There are other shops in Fabbriche di Vallico - 5 minutes drive downhill, and a giant Leclerc supermarket in Galliciano (20 minutes drive).

You are of course welcome to make use of the Institute's cooking facilities whenever you want; in fact why not cook a lovely dinner for four demonstrating the cuisine of your country? There is a huge downstairs kitchen 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 very much encouraged to try. There are also two kitchens in the adjacent Doctor's house which will be rented for the duration of the conference.

On the first evening a special buffet dinner will be provided. Later in the week the Institute's 15th Century pizza oven will be pressed into service. The rest of the time we will make use of the excellent local restaurants - these are mostly incredibly cheap. Given the large number of people staying at the Institute, people are encouraged to break up into at least two groups, although Da Sandra is large enough to handle everyone. Ask Mike to make reservations for you if you don't speak Italian.

LIST OF LOCAL RESTAURANTS

- Da Sandra (0583 761289 on the road between Fabbriche di Vallico and Vallico Sotto).

- Il Canapale (0583 761829, Vallico Sopra)
- Al Laghetto (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)
- Alta Matanna (0584 776005)
- Mulino Biologico (Fabbriche di Vallico)

RESTAURANTS SLIGHTLY FURTHER AFIELD

- Circolo dei Forestieri, Bagni di Lucca
- Antica Trattoria dell'Eremita, Vergemoli
- LOTS MORE - ASK

10 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). Starting in June 2006 there will be a weekly film to which the whole valley will be invited (providing we can buy more chairs before then). During the conference you are welcome to use the projectors and it is expected that movies will be shown most nights. 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 - Alan Aspuru-Guzik has already volunteered..

11 SUMMER SCHOOL

Note that the conference will be followed by a Summer School the following week, taught by Richard Needs, Mike Towler, Neil Drummond and Pablo Lopez Rios. For reference, here is the draft schedule.

Sunday 30th July

ARRIVALS

~8.30pm : Buffet dinner in the Institute garden.

Monday 31st July

8.30am : Mike Towler - "Quantum Monte Carlo : the basics. Overview of everything. Why QMC? Basic MC integration/VMC/DMC theory. Many-electron wave functions - aperiodic and periodic. Basic solid-state ideas - reciprocal space, k points etc. Idea of wave function optimization Representation of orbitals. Basis sets. Spin. Excited states. Total energy." (2.5 hours)

11am : BREAK

11.30am : Mike Towler - "An introduction to the CASINO program" (1 hour)

1pm LUNCH

EXCURSION - Trip to Alta Matanna.

PRACTICAL SESSION -

Distribution, setup and compilation of the CASINO program (MDT)

8.30PM DINNER

Tuesday 1st August

8.30am : Pablo Lopez Rios - "Statistical analysis of VMC results. Basic DMC -
how to run a calculation. How to extract and analyze DMC results.
Serial correlation. Timestep optimization. Correlation time.
Reblocking. Use of graphit program. Other statistical issues."
(1 hour)
9.30am : Alexander Badinski - "Pseudopotentials for quantum Monte Carlo"
(1 hour)
10.30am : BREAK
11am : Richard Needs - "Solid state calculations. Interactions and
finite size effects" (2 hours)

1pm Lunch

EXCURSION/ACTIVITY

PRACTICAL SESSION -

Basic use of CASINO program - simple VMC, DMC calculations (MDT)

8.30pm DINNER

Wednesday 2nd August

8.30am : Neil Drummond - "Jastrow factors and wave function optimization"
(2 hours)
10.30am : BREAK
11am : Pablo Lopez Rios - "Orbital optimization, multideterminants and
backflow, with numerical results" (2 hours)

1pm LUNCH

EXCURSION/ACTIVITY

PRACTICAL SESSION

- Wave function optimization with CASINO (NDD)

8.30pm DINNER

Thursday 3rd August

11.00am : Neil Drummond - "Advanced diffusion Monte Carlo. Timestep errors.
Green's function modifications. Fixed-node
approximation. Wave function nodes. Fermion sign
problem (release node and fermion Monte Carlo,
optimizing the nodes). Expectation
values in DMC. Future walking etc. Population
explosions. Idea of reptation and path-integral
Monte Carlo." (2 hours)
10.30am : BREAK
11.00am : Mike Towler - "Scaling with system size. Localized orbitals
and localized basis sets (Gaussians/blips).

All-electron calculations. Heavy atoms -
timestep errors. Forces. Non-collinear
spins and complex wave function mode" (2 hours)

1pm LUNCH

EXCURSION/ACTIVITY

PRACTICAL SESSION

- Advanced use of the CASINO program (PLR)

8.30pm DINNER

Friday 4th August

8.30am : Mike Towler - "Expectation values other than the total
energy computable with CASINO" (1 hour)
9.30am : Pablo Lopez Rios - "Applications : electron-only systems (fluid phase,
Wigner crystals etc.) Electron-hole systems.
(1 hour)
10.30am : BREAK
11.00am : Neil Drummond - "Applications : systems with atoms" (1 hour)
12.30am : Mike Towler - "Conclusions and open problems" (1 hour)

1pm LUNCH

EXCURSION/ACTIVITY

PRACTICAL SESSION

- Trial wave function generation with other programs (CRYSTAL/PWSCF/CASTEP etc.)

8.30pm DINNER

Saturday 5th August

MORNING - Exercises with CASINO and QMC exam (with prizes)

AFTERNOON/DINNER - Long distance excursion e.g. to Cinque Terre

Sunday 6th August

DEPARTURES

12 FINAL THOUGHT

HAVE FUN AT THE TOWLER INSTITUTE!