

How can QMC become
mainstream?
or, why is the community so small?

David Ceperley's reasons (1996)

1. We need forces, dummy!
2. Try getting O₂ to bind at the variational level.
3. How many graduate students lives have been lost optimizing wavefunctions?
4. It is hard to get 0.01 eV accuracy by throwing dice.
5. Most chemical problems have more than 50 electrons.
6. Who thought LDA or HF pseudopotentials would be any good?
7. How many spectra have you seen computed by QMC?
8. QMC is only exact for energies.
9. Multiple determinants. We can't live with them, we can't live without them.
10. After all, electrons are fermions.
11. Electrons move.
12. QMC isn't included in Gaussian 90. Who programs anyway?

Mike Towler's responses:

http://www.psi-k.org/newsletters/News_60/Highlight_60.pdf

What we get with a bigger community

Good things:

- More innovations
- Larger mindshare
- More students (some will be very good)
- Can support specialists (coding)
- Things working in a robust way (lots of eyes)
- Increased funding/more jobs
- Whittle down number of codes
- Regularity and reproducibility

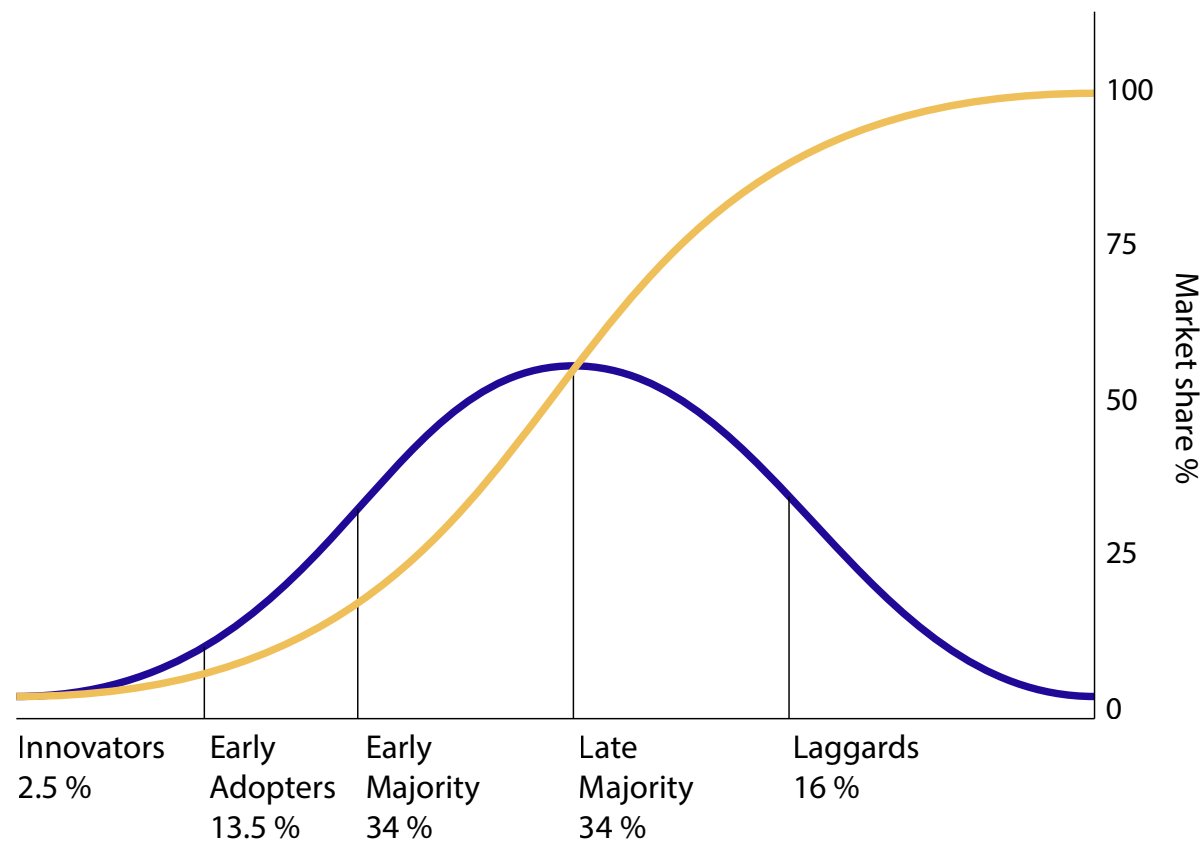
Bad things:

- Harder to keep up
- Different group dynamics
- Possible 'superstar' culture

Neutral thing:

- Segregation into user community and developer community
- There will be people who have no idea what's going on
- More competition for science and for computers/resources

Who are our early adopters?



Predict stability of structures

Force fields

Activation energies

Defect physics

Benchmarks of correlation energies

Better shot at strongly correlated systems

Equations of state

Phase diagram (high pressure, etc)

Larger systems > 50 electrons

Excitations/excitonic properties

Spectra (vibrational/electronic)

Artificial photosynthesis (spectra)

Systems where correlation effects are important locally (and can be embedded)

Model systems

Systems where static/dynamic correlations are important

Catalysis (activation energies, dH)

Positronic systems

Drug discovery

People who have a lot of computers

Anyone who's currently using a quantum chemistry code

Diffusion of Innovation, Everett M. Rogers

Five stages of the adoption process

Stage	Definition
Knowledge	The individual is first exposed to an innovation, but lacks information about the innovation. During this stage the individual has not yet been inspired to find out more information about the innovation.
Persuasion	The individual is interested in the innovation and actively seeks related information/details.
Decision	The individual takes the concept of the change and weighs the advantages/disadvantages of using the innovation and decides whether to adopt or reject the innovation. Due to the individualistic nature of this stage, Rogers notes that it is the most difficult stage on which to acquire empirical evidence. ^[11]
Implementation	The individual employs the innovation to a varying degree depending on the situation. During this stage the individual also determines the usefulness of the innovation and may search for further information about it.
Confirmation	The individual finalizes his/her decision to continue using the innovation. This stage is both intrapersonal (may cause cognitive dissonance) and interpersonal, confirmation the group has made the right decision.

Change agents

Trust & commonality of viewpoint

DFT languished, but Pople brought it to the chemists ~1990/1991

Carr-Parinello in physics, brought dynamics

Can never predict when something goes from unfashionable to fashionable, takes time

In DFT, the first MD calculations were important

DMFT community has done a better job, don't know how.

Benchmark problems that show definitively that the method works

Solving a problem that hasn't been solved very well (electron gas was like that)

Non-users can have access quickly to the calculation

Visibility

No one knows about QMC, so there isn't much common ground

Sometimes make promises that we can't keep

People don't like error bars

Quantum simulation menu

Density functional Theory.....100 node-hours

*Total energies within 1-2 eV
Easily interpretable band structures
Choice of functional*

Hybrid DFT.....1000 node-hours

*Total energies within 0.5 eV
Similar band structure as regular DFT, better gaps
Occasional spectacular failures*

Fixed node diffusion Monte Carlo..50000 node-hours

*Total energies within 0.1 eV
Only includes a gap
Bring your own trial wave function*

Full CI quantum Monte Carlo.....500000 node-hours

*Total energies better than 0.1 eV
Exact within the basis*

Node-hours are controversial!

What should the menu have on it?

What can be calculated

total energy, gap, one-electron Green function, density, forces, dynamic structure factor, thermal properties, entanglement entropy, Hessian of the atomic position, imaginary/real time correlation functions, output of experimental machine, spectroscopic data, response functions/susceptibilities (magnetic, charge, superconductivity),

How accurate those things are

How long it takes to calculate

changes quickly, doesn't need to be incredibly accurate
(possibly in student-months)

What would it take for people to provide this?

Generally response is less than enthusiastic. Too many man-hours.

Other communities have done this—structure prediction blind test (crystal and protein)

Combinatoric,

Relative advantage: the degree to which an innovation is perceived as better than the idea it supersedes.

Compatibility: the degree to which an innovation is perceived as being consistent with the existing values, past experiences, and needs of potential adopters.

Complexity: the degree to which an innovation is perceived as difficult to understand and use.

Trialability: the degree to which an innovation may be experimented with on a limited basis.

Observability: the degree to which the results of an innovation are visible to others.

Relative advantage

the degree to which an innovation is perceived as better than the idea it supersedes.

Strengths

Correct forces

Correlations for larger systems

Error bars (actual)

Variational energies

Can actually get the right answer

Systematically improvable (in principle)

When you get the right answer, you can understand why.

Low memory requirements

Massive parallelism

Generality—works for many different systems

Many-body description

Can crack bottlenecks (CASSCF, basis sets)

Often very simple to code

Weaknesses

No band structure

Error bars (perceived)

Understanding stochasticity

Poor documentation

DFT is often ‘good enough’

Costs a lot of computer time

Small energy differences are difficult

Dynamics are hard to do

Almost always some uncontrolled errors

One number is not a diagram (numbers/core hour is low)

Phonon dispersions, absorption, etc are hard to calculate

Compatibility

the degree to which an innovation is perceived as being consistent with the existing values, past experiences, and needs of potential adopters.

Strengths

Total energies are central

Effective masses

One-particle GF

Response functions (depends on MC)

Temperature

Weaknesses

Band structures

Not integrated into standard procedures/codes (but could be)

Many people think in spectra/Fermi surfaces

Theory: effective Fermi surface+ some physics

Quasiparticle

Wave function analysis

There's little you can do only with DMC (no unique properties)

Complexity

the degree to which an innovation is perceived as difficult to understand and use.

Strengths

Weaknesses

Pseudopotentials

Statistics

Often interface to another code

Trialability

the degree to which an innovation may be experimented with on a limited basis.

Strengths

Weaknesses

One cannot run MC for any given system easily

No GUI

No QMC for Dummies (overview of methods)

Many choices (jastrow factor, basis set, method)

Observability

the degree to which the results of an innovation are visible to others.

Strengths

People trust/pay attention to
QMC results

Weaknesses

Not talked about much in conferences
Lots of method development, not as much
application development
Not taught in courses/textbooks
Scattered web presence
Nothing in Wikipedia

What are the current challenges?

Target audience is unclear

Cooperation with other communities, communicating strengths and understanding target audience

For some problems, accuracy is not quite good enough in standard FN-DMC

We'd like to be around 3x more accurate. (we are already 10x more accurate than DFT)

While in principle systematically improvable, in practice difficult.

Finite size effects.

Where will we be in 5 years?

Make calculation better button in VASP

Proper quantum chemistry for solids (for proper definition of proper)

Quickly calculate formation energies of 10's of systems within a few days

Reliable forces

Effective band structure or Greens function calculated efficiently

Better worked out standards

Automated capabilities for some problems

Coherence around a small number of codes (~2 DMC codes for ex.)

Standard benchmarking set for solids (like Luke Shulenberger)

Using modern computing platforms

New review paper

What do we need? Infrastructure? Money?

Bigger computers

More time

More money

Money for software-only developments

Long-term funding

Permanent positions available

Good politicians

A way to form an identity, cohesion

Buy in from cousin communities

Workshops to blend communities (Many-body computational community and electronic structure)

Summer schools for students (bridge the instruction gap)