

Superconductivity the Next “industrial revolution”

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About the Author

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- Visiting Professor at Department of Physics in Northeastern University, Boston, US
- Docent at Department of Physics in Tampere University of Technology, Finland
- Head of Computational Quantum Physics Laboratory at TUT

- Research interest: Computational methods of surface science to determine geometrical and electronic structure of surface. Angle Resolved photoemission of high T_c superconductors.

- International refereed publications:
<http://alpha.cc.tut.fi/~lindroos/publications.html>



Background

- Superconductivity intrigues researchers across the world – from Nobelists to dissertationists.
- Whoever solves the issue of how to turn superconductivity into a practice that **allows the transfer of energy with almost no electrical resistance** in regular or financially feasible conditions, will take a place in the history of science.



Superconductivity and the Possibilities



Photograph by Rama, Wikimedia Commons, Cc-by-sa-2.0-fr



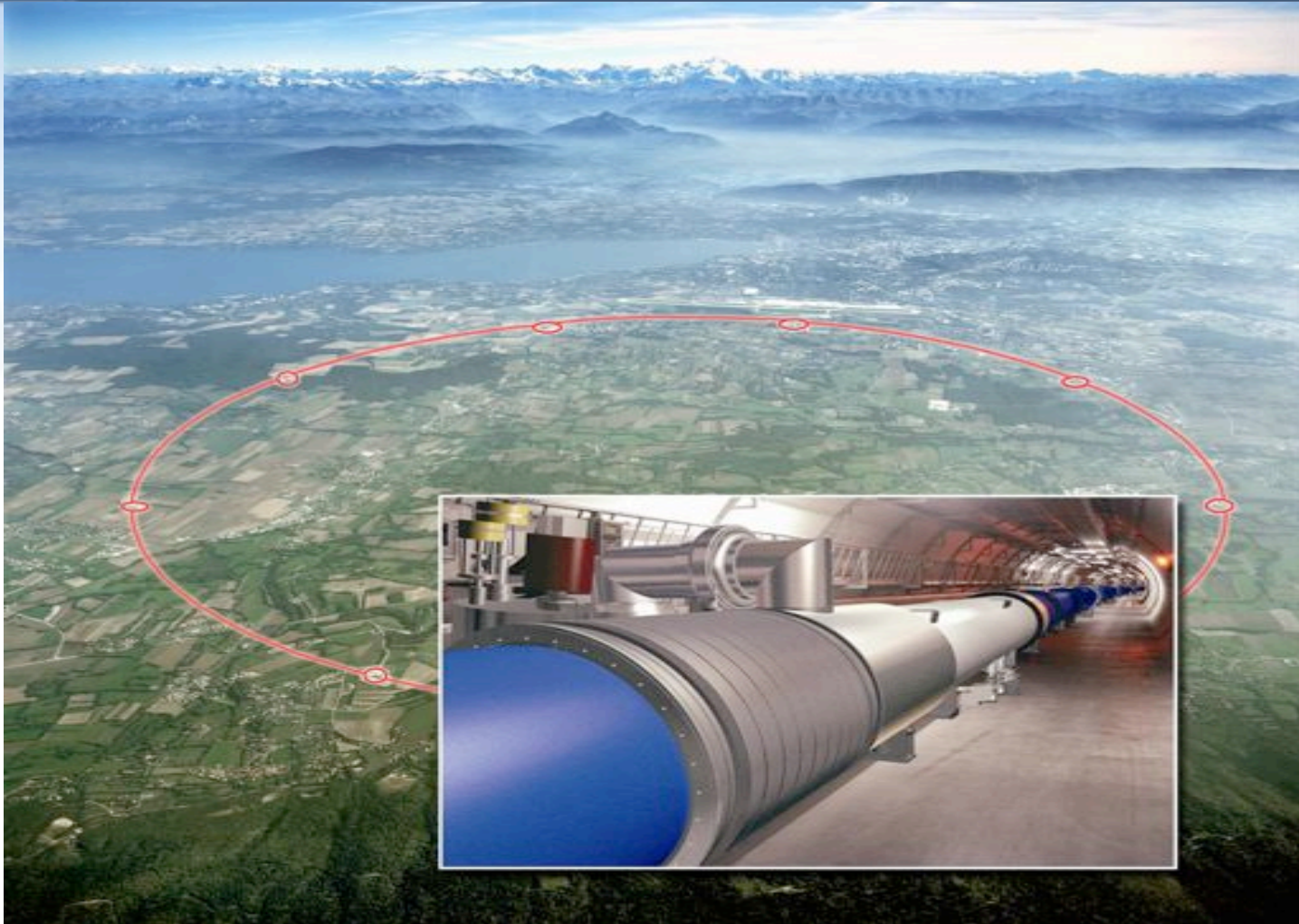
Superconductivity and the Possibilities



Source: <http://www.supertightstuff.com/wp-content/uploads/2009/04/jr-maglev.jpg>



Superconductivity and the Possibilities



Source: <http://www.lbl.gov/publicinfo/newscenter/features/08/06/12/hires/LHC-CERN-over.jpg>

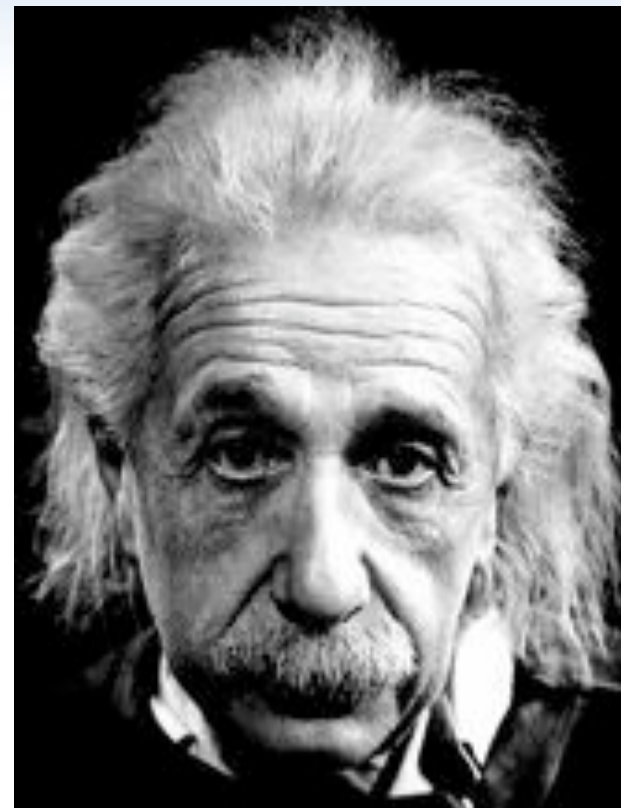


Research of the Origin of Superconductivity

- Today we have two main lines of research
 - A highly complex theoretical many body modeling
 - Empirical research on properties of SC materials
- Theories on the origin of superconductivity predict properties for experimental testing.
- If predictions and experiments do not agree theories are discarded as invalid.



"The solutions to the problems we face today cannot be solved on the same level of thinking we were at when we created them."



Source: <http://dyslexiavictoria.files.wordpress.com/2009/06/albert-einstein1.jpg>



My Research = Photoemission

- Obtaining a comprehensive picture of the unconventional superconductors relies very much on electronic spectrometers based on injection or extraction of electrons from superconducting samples.
- For such picture we have to run computations with multiple variables, check the results with experimental predictions and slightly adjust the combinations of parameters and run again.

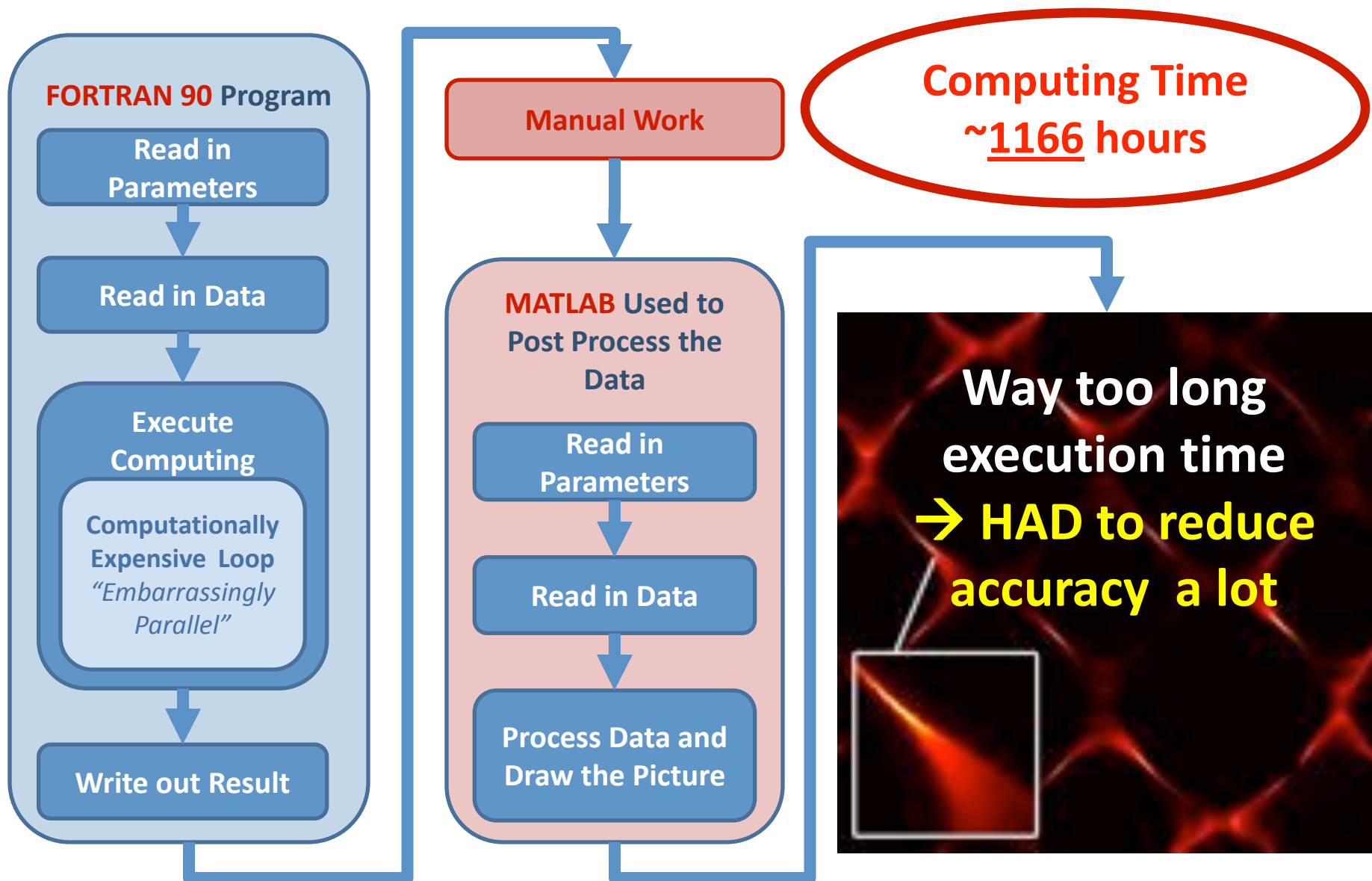


The One Step Equation for Photoemission Intensity

$$I(\mathbf{k}_{\parallel}, E_f) = -\frac{1}{\pi} \Im \langle \mathbf{k}_{\parallel}, E_f | G_2^+ \Delta G_1^+ \Delta^\dagger G_2^- | \mathbf{k}_{\parallel}, E_f \rangle$$

- High-Performance Computers (HPC) with Message Passing Interface (MPI) was tested at NERSC
 - Scalability problems
 - HPC & queuing, MPI & complexity → **frustration!**
 - Need for a simple, scalable and fast solution
- The equation is “Embarrassingly parallel”
 - every \mathbf{k}_{\parallel} value can be computed independently





“Insanity – continuing to do things the way they have always been done and expecting the results to be significantly different”.

- Dr. W. Edwards Deming, the 'father of quality' -



MATLAB Program that
Calls Automatically
FORTRAN 90 and Post-
Process the Result

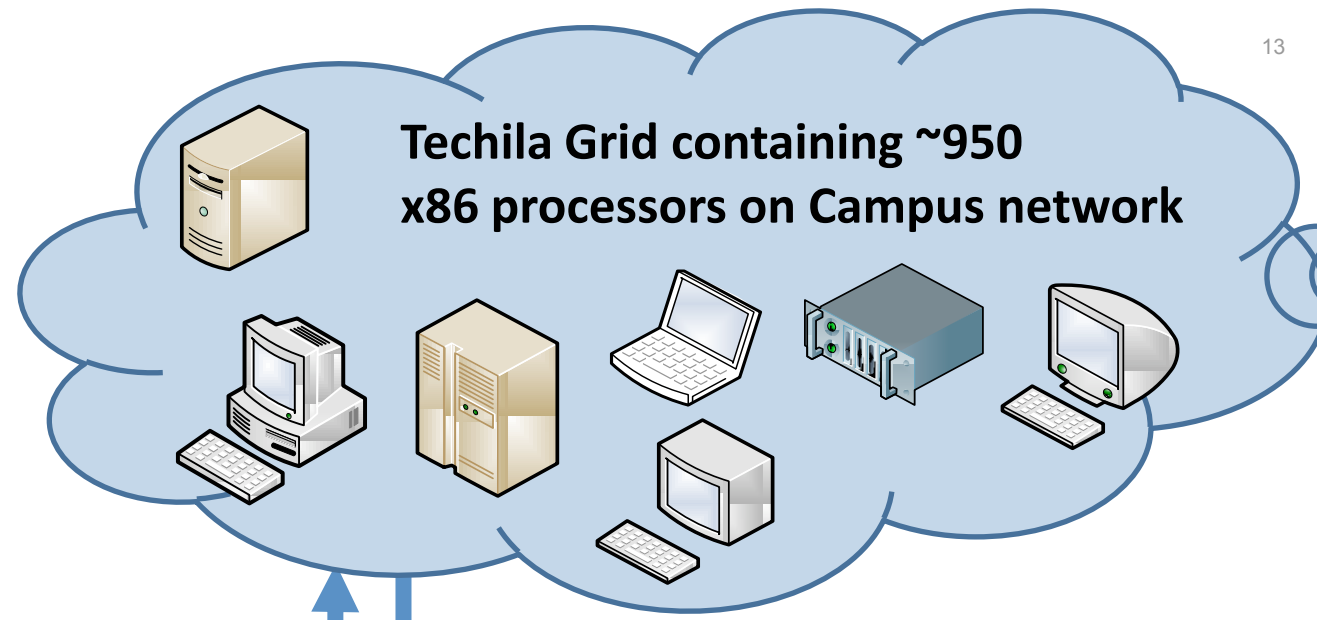
Read in Parameters

Read in Data

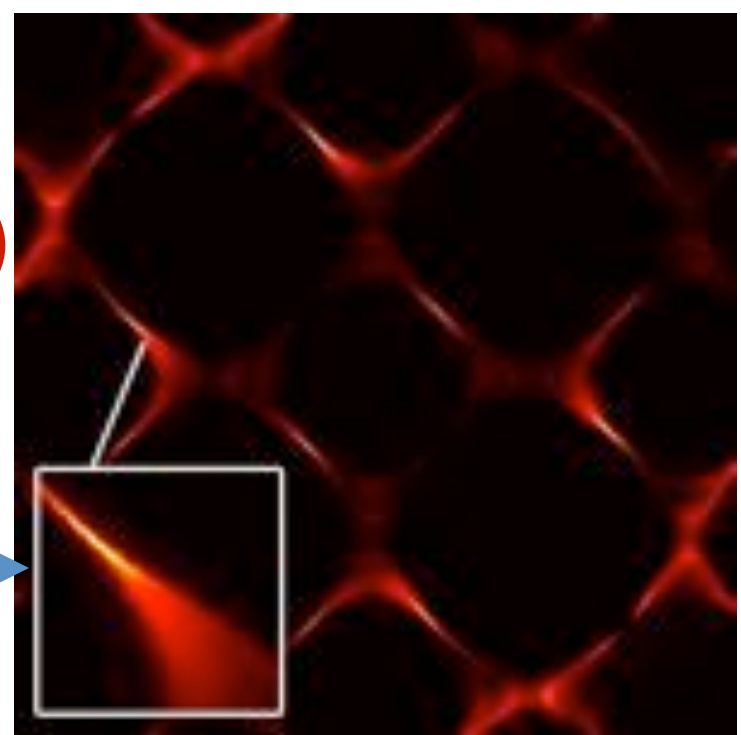
Distribute FORTRAN
Computation to
GRID

Get Results from the
GRID

Process Results and
Draw the Picture



**Computing Time
~2½ hours**



Examples of Computing Accuracy Versus Time

- Next five pages will demonstrate what it means when accuracy is increased in our computations.
- We start from 50x50 matrix that equals 2.500 independent calculations and we end with 256 times more accurate 800x800 matrix.
- As mentioned earlier we have to run computations with multiple variables, check the results with experimental predictions and slightly adjust the combinations of parameters and run again → **tens of computations to be completed.**



50x50 Matrix

Acceleration factor = 9690.84%.

CPU time used 0 d 3 h 31 m 35 s.
Real time used 0 d 0 h 2 m 11 s.

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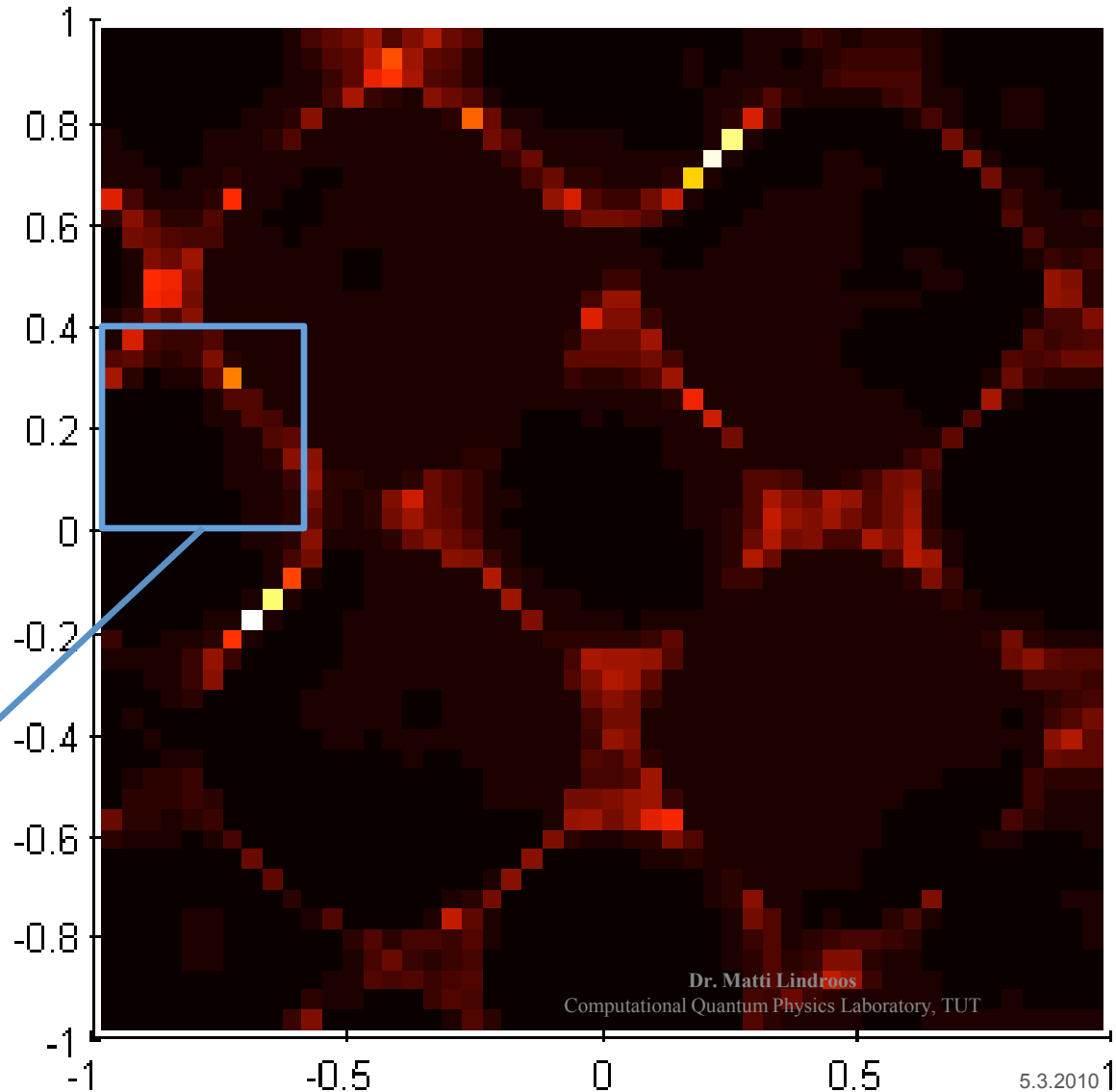
Project Statistics:

96 nodes participated

Avg efficiency per job: 96.79%

CPU Time per job: 49.786s (avg)

70.124s (max)



100x100 Matrix

Acceleration factor = 22599.63%.

CPU time used 0 d 16 h 53 m 13 s.

Real time used 0 d 0 h 4 m 29 s.

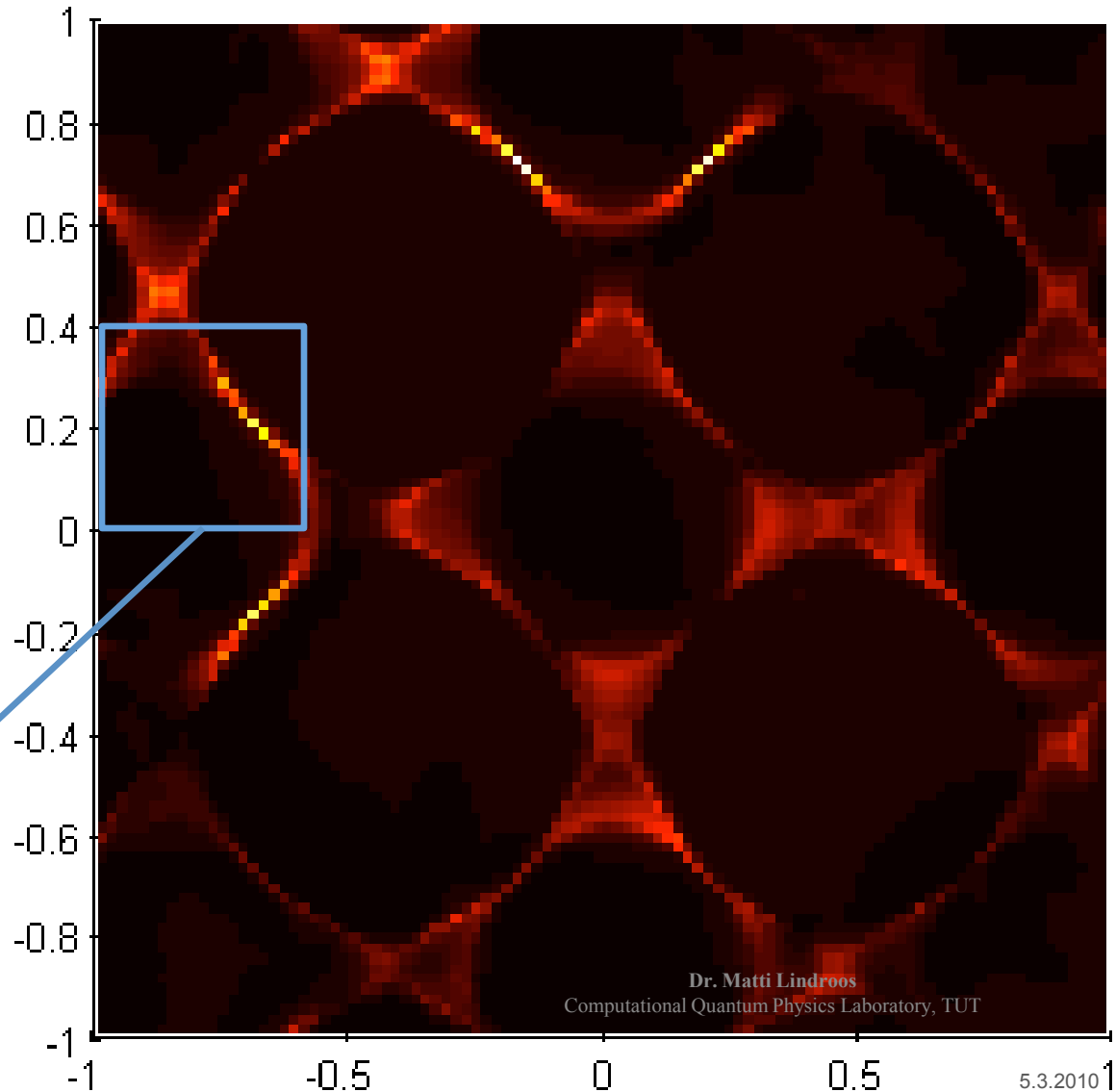
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Project Statistics:

197 nodes participated

Avg efficiency per job: 95.90%

**CPU Time per job: 60.192s (avg)
 138.186s (max)**



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200x200 Matrix

Acceleration factor = 31498.87%.

CPU time used 2 d 21 h 23 m 6 s.

Real time used 0 d 0 h 13 m 13 s.

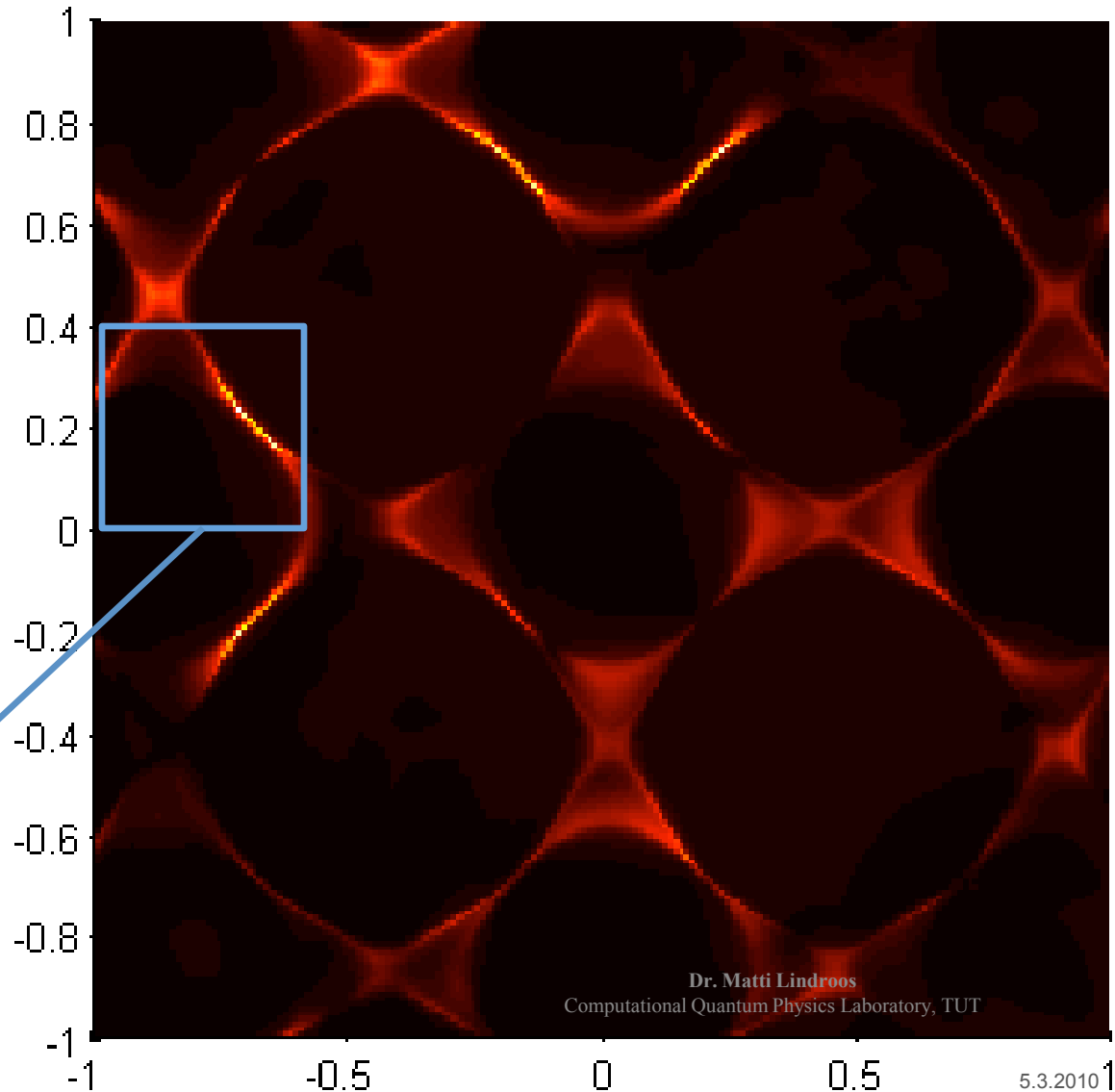
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Project Statistics:

224 nodes participated

Avg efficiency per job: 95.33%

**CPU Time per job: 65.406s (avg)
 138.686s (max)**



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400x400 Matrix

Acceleration factor = 38146.36%.

CPU time used 11 d 14 h 21 m 45 s.
Real time used 0 d 0 h 43 m 47 s.

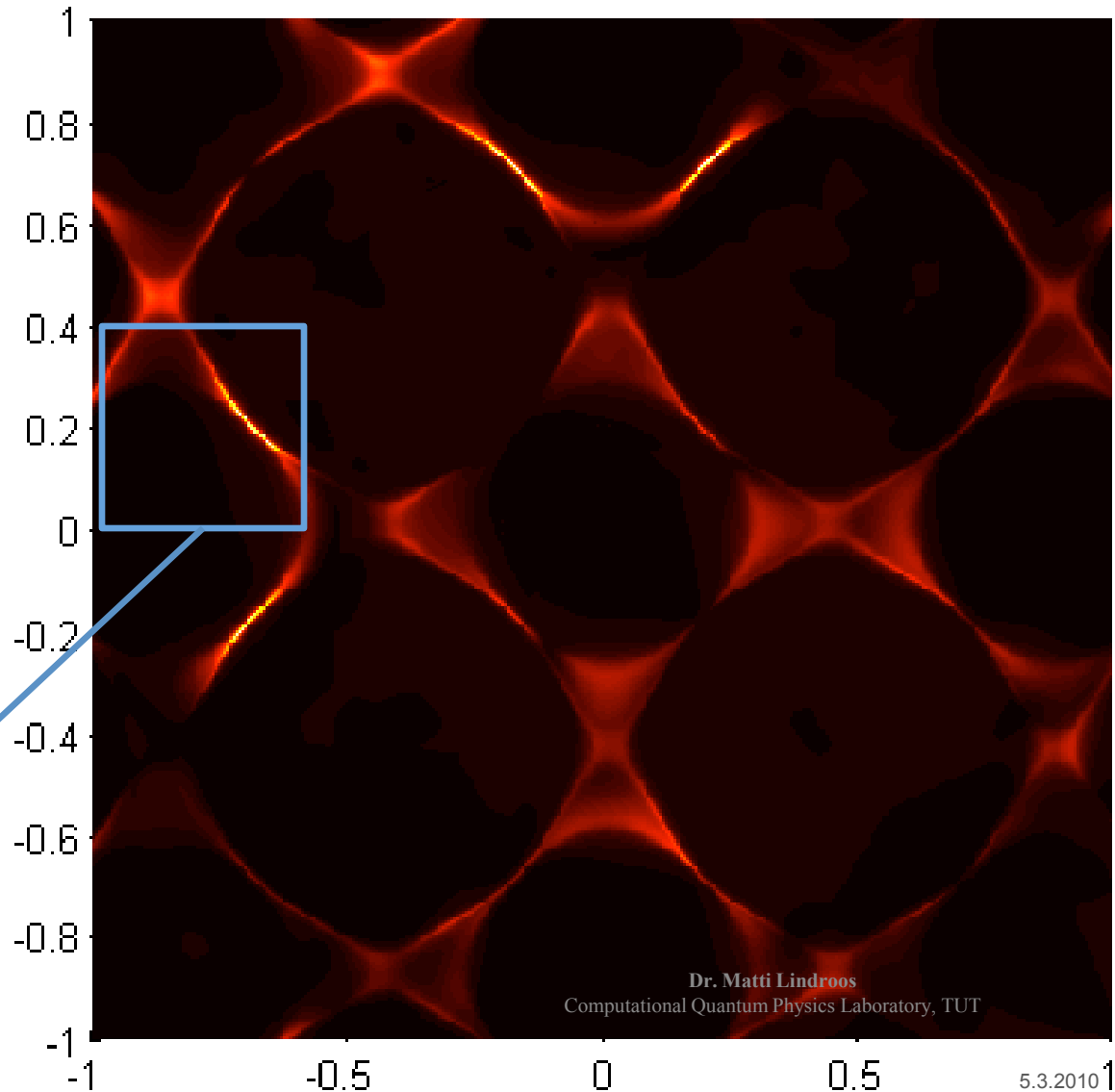
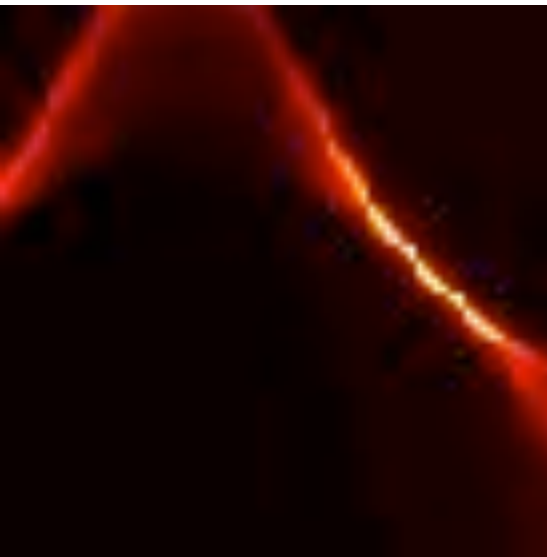
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Project Statistics:

269 nodes participated

Avg efficiency per job: 95.05%

CPU Time per job: 67.541s (avg)
139.484s (max)



800x800 Matrix

Acceleration factor = 45622.72%.

CPU time used 48 d 14 h 25 m 15 s.
Real time used 0 d 2 h 33 m 24 s.

#####

Project Statistics:

329 nodes participated

Avg efficiency per job: 95.45%

CPU Time per job: 67.541s (avg)
138.564s (max)

