PyProp - A Python Framework for Propagating the Time Dependent Schrödinger Equation

Tore Birkeland

Department of Mathematics, University of Bergen

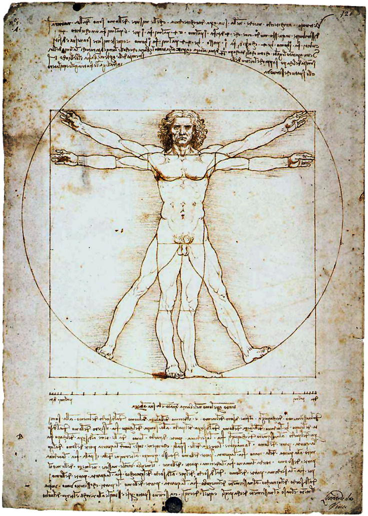
December 18, 2009

UNIVERSITY OF BERGEN

Underlying Goal

Study the behaviour of atoms and molecules

Length Scale

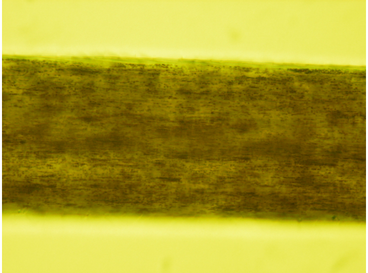


10^{0}m	Humans
10^{-2}m	Golf balls
10^{-4}m	Width of human hair
10^{-6}m	Cells
10^{-8}m	Vira
10^{-10}m	Atoms

Length Scale

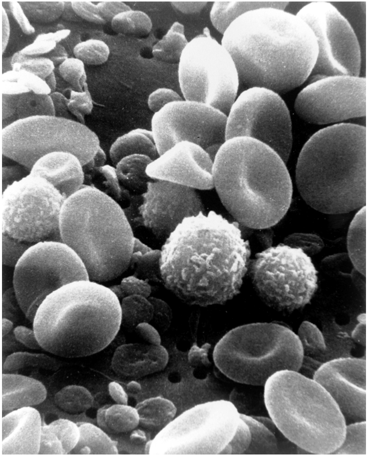
10^{0}m	Humans
10^{-2}m	Golf balls
10^{-4}m	Width of human hair
10^{-6}m	Cells
10^{-8}m	Vira
10^{-10}m	Atoms

Length Scale



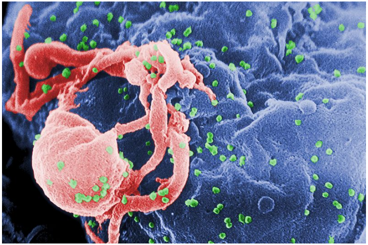
10^{0}m	Humans
10^{-2}m	Golf balls
10^{-4}m	Width of human hair
10^{-6}m	Cells
10^{-8}m	Vira
10^{-10}m	Atoms

Length Scale



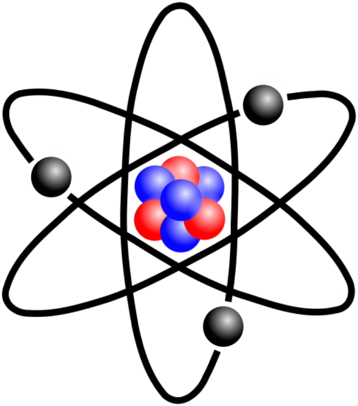
10^0m	Humans
10^{-2}m	Golf balls
10^{-4}m	Width of human hair
10^{-6}m	Cells
10^{-8}m	Vira
10^{-10}m	Atoms

Length Scale



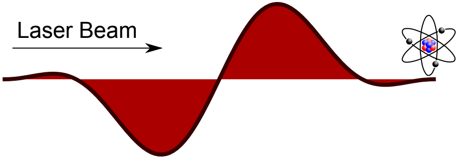
10^{0}m	Humans
10^{-2}m	Golf balls
10^{-4}m	Width of human hair
10^{-6}m	Cells
10^{-8}m	Vira
10^{-10}m	Atoms

Length Scale



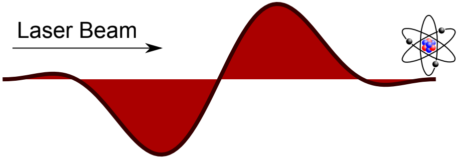
10^{0}m	Humans
10^{-2}m	Golf balls
10^{-4}m	Width of human hair
10^{-6}m	Cells
10^{-8}m	Vira
10^{-10}m	Atoms

How?



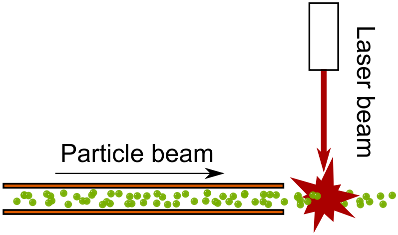
- Atoms are smaller than the wavelength of light
- Any observation leads to a modification of the system
- It is not possible to directly observe what is going on
- Need theoretical models and calculations to match experiments

How?



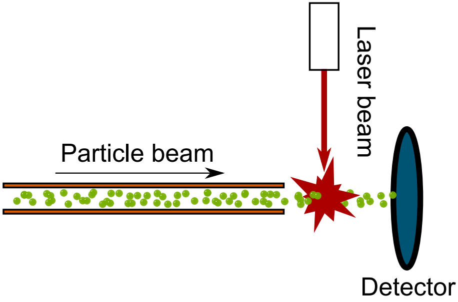
- Atoms are smaller than the wavelength of light
- Any observation leads to a modification of the system
- It is not possible to directly observe what is going on
- Need theoretical models and calculations to match experiments

How?



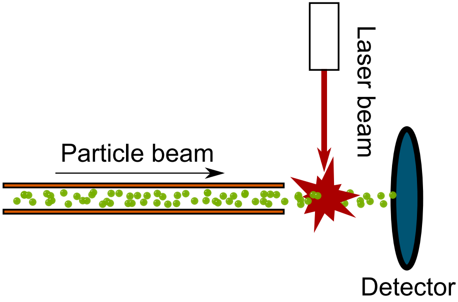
- Atoms are smaller than the wavelength of light
- Any observation leads to a modification of the system
- It is not possible to directly observe what is going on
- Need theoretical models and calculations to match experiments

How?



- Atoms are smaller than the wavelength of light
- Any observation leads to a modification of the system
- It is not possible to directly observe what is going on
- Need theoretical models and calculations to match experiments

How?



- Atoms are smaller than the wavelength of light
- Any observation leads to a modification of the system
- It is not possible to directly observe what is going on
- Need theoretical models and calculations to match experiments

Numerical Experiment

Simulation of an experimental setup on a computer

1. An atomic/molecular system is in an initial state
2. The system interacts with an external force
   - Interaction with radiation (laser)
   - Collision with another atom/ion/molecule
3. The final state of the system is analyzed to compare with experiments

The goal of this thesis is to perform steps 1 and 2 and simplify step 3 for a wide range of problems

Numerical Experiment

Simulation of an experimental setup on a computer

1. An atomic/molecular system is in an initial state
2. The system interacts with an external force
   - Interaction with radiation (laser)
   - Collision with another atom/ion/molecule
3. The final state of the system is analyzed to compare with experiments

The goal of this thesis is to perform steps 1 and 2 and simplify step 3 for a wide range of problems

Numerical Experiment

Simulation of an experimental setup on a computer

1. An atomic/molecular system is in an initial state
2. The system interacts with an external force
   - Interaction with radiation (laser)
   - Collision with another atom/ion/molecule
3. The final state of the system is analyzed to compare with experiments

The goal of this thesis is to perform steps 1 and 2 and simplify step 3 for a wide range of problems

Numerical Experiment

Simulation of an experimental setup on a computer

1. An atomic/molecular system is in an initial state
2. The system interacts with an external force
   - Interaction with radiation (laser)
   - Collision with another atom/ion/molecule
3. The final state of the system is analyzed to compare with experiments

The goal of this thesis is to perform steps 1 and 2 and simplify step 3 for a wide range of problems

Numerical Experiment

Simulation of an experimental setup on a computer

1. An atomic/molecular system is in an initial state
2. The system interacts with an external force
   - Interaction with radiation (laser)
   - Collision with another atom/ion/molecule
3. The final state of the system is analyzed to compare with experiments

The goal of this thesis is to perform steps 1 and 2 and simplify step 3 for a wide range of problems

Outline

- Overview of the thesis
- Introduction to Quantum Mechanics
- Solving the Time Dependent Schrödinger Equation on a computer
- How PyProp is a flexible solver
- Applying PyProp to laser ionization of Helium

Thesis Overview

Development and application of PyProp

- Computer Science - Software design and implementation
- Mathematics - Numerical methods
- Physics - Applications

What is PyProp?

Framework for solving the Time Dependent Schrödinger Equation

- Goals
  - Flexibility
  - Performance
- Research tool, not QM@Home
  - Common tasks automated
  - Difficult tasks possible
- Free Software (GPL) http://pyprop.googlecode.com

What is PyProp?

Framework for solving the Time Dependent Schrödinger Equation

- Goals
  - Flexibility
  - Performance
- Research tool, not QM@Home
  - Common tasks automated
  - Difficult tasks possible
- Free Software (GPL) http://pyprop.googlecode.com

What is PyProp?

Framework for solving the Time Dependent Schrödinger Equation

- Goals
  - Flexibility
  - Performance
- Research tool, not QM@Home
  - Common tasks automated
  - Difficult tasks possible
- Free Software (GPL) http://pyprop.googlecode.com

What is PyProp?

Framework for solving the Time Dependent Schrödinger Equation

- Goals
  - Flexibility
  - Performance
- Research tool, not QM@Home
  - Common tasks automated
  - Difficult tasks possible
- Free Software (GPL) http://pyprop.googlecode.com

Scientific Results

1. T. Birkeland, M. Førre, J. P. Hansen and S. Selstø, *Dynamics of H_{2p} ionization in ultrashort strong laser pulses*, J. Phys. B At. Mol. Opt. Phys, **37** 4205-4219 (2004)
2. T. Birkeland and T. Sørevik *Parallel Redistribution of Multidimensional Data* Proceedings ParCo 2007 Conference NIC Series Volume **38**, (2007)
3. V. Popsueva, R. Nepstad, T. Birkeland, M. Førre, J. P. Hansen, E. Lindroth and E. Waltersson, *Structure of lateral two-electron quantum dot molecules in electromagnetic fields* Physical Review B, **76**, 035303 (2007)
4. L. Sælen, I. Sundvor, T. Birkeland, S. Selstø, and M. Førre, *Classical and quantum-mechanical investigation of the role of nondipole effects on the binding of a stripped HD^{2+} molecule* Physical Review A, **76**, 013415 (2007)
5. T. Sørevik, T. Birkeland and G. Okša, *Numerical solution of the 3D time dependent Schrödinger equation in spherical coordinates: Spectral basis and effects of split-operator technique* Journal of Computational and Applied Mathematics, **225**, 56-67 (2007)
6. C. R. Calvert, T. Birkeland, R. B. King, I. D. Williams and J. F. McCann, *Quantum chessboards in the deuterium molecular ion* J. Phys. B: At. Mol. Opt. Phys., **41**, 205504 (2008)
7. T. Birkeland and T. Sørevik, *Parallel Pseudo-spectral Methods for the Time Dependent Schrödinger Equation* Parallel Computing: Numerics, Applications, and Trends R. Trobec, M Vajteršic and P. Zinterhof (ed.) 261-279 (2009)
8. C. R. Calvert, R. B. King, T. Birkeland. J. D. Alexander, J. B. Greenwood, W. A. Bryan, W. R. Newell, D. S. Murphy, J. F. McCann and I. D. Williams, *Pathways to state-selective control of vibrational wavepackets in the deuterium molecular ion* Journal of Modern Optics, **56** 1060-1069 (2009)
9. T. Birkeland and R. Strand, *How to Understand Nano Images*, Techne: Research in Philosophy and Technology, in print (2009)
10. R. Strand and T. Birkeland, *The Science and Politics of Nano Images* Nano meets Macro: Social Perspectives on Nanoscale Sciences and Technologies, (2009)
11. L. Sælen, T. Birkeland, N. Sisourat, A. Dubois and J. P. Hansen, *Full 3D ab initio studies of interference effects in high-energy ion-molecule collisions* Proceedings of ICPEAC XXVI, in print (2009)
12. L. Sælen, T. Birkeland, N. Sisourat, A. Dubois and J. P. Hansen, *Non perturbative treatment of single ionization of H_2 by fast, highly charged ion impact*, submitted for publication (2009)
13. T. Birkeland, R. Nepstad and M. Førre, *Multiphoton Double Ionization in Helium Driven by Intense XUV Attosecond Pulses*, to be submitted

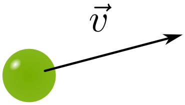
Scientific Results

1. T. Birkeland, M. Førre, J. P. Hansen and S. Selstø, *Dynamics of H_{2p} ionization in ultrashort strong laser pulses*, J. Phys. B At. Mol. Opt. Phys, **37** 4205-4219 (2004)
2. T. Birkeland and T. Sørevik *Parallel Redistribution of Multidimensional Data* Proceedings ParCo 2007 Conference NIC Series Volume **38**, (2007)
3. V. Popsueva, R. Nepstad, T. Birkeland, M. Førre, J. P. Hansen, E. Lindroth and E. Waltersson, *Structure of lateral two-electron quantum dot molecules in electromagnetic fields* Physical Review B, **76**, 035303 (2007)
4. L. Sælen, I. Sundvor, T. Birkeland, S. Selstø, and M. Førre, *Classical and quantum-mechanical investigation of the role of nondipole effects on the binding of a stripped HD^{2+} molecule* Physical Review A, **76**, 013415 (2007)
5. T. Sørevik, T. Birkeland and G. Okša, *Numerical solution of the 3D time dependent Schrödinger equation in spherical coordinates: Spectral basis and effects of split-operator technique* Journal of Computational and Applied Mathematics, **225**, 56-67 (2007)
6. C. R. Calvert, T. Birkeland, R. B. King, I. D. Williams and J. F. McCann, *Quantum chessboards in the deuterium molecular ion* J. Phys. B: At. Mol. Opt. Phys., **41**, 205504 (2008)
7. T. Birkeland and T. Sørevik, *Parallel Pseudo-spectral Methods for the Time Dependent Schrödinger Equation* Parallel Computing: Numerics, Applications, and Trends R. Trobec, M Vajteršic and P. Zinterhof (ed.) 261-279 (2009)
8. C. R. Calvert, R. B. King, T. Birkeland. J. D. Alexander, J. B. Greenwood, W. A. Bryan, W. R. Newell, D. S. Murphy, J. F. McCann and I. D. Williams, *Pathways to state-selective control of vibrational wavepackets in the deuterium molecular ion* Journal of Modern Optics, **56** 1060-1069 (2009)
9. T. Birkeland and R. Strand, *How to Understand Nano Images*, Techne: Research in Philosophy and Technology, in print (2009)
10. R. Strand and T. Birkeland, *The Science and Politics of Nano Images* Nano meets Macro: Social Perspectives on Nanoscale Sciences and Technologies, (2009)
11. L. Sælen, T. Birkeland, N. Sisourat, A. Dubois and J. P. Hansen, *Full 3D ab initio studies of interference effects in high-energy ion-molecule collisions* Proceedings of ICPEAC XXVI, in print (2009)
12. L. Sælen, T. Birkeland, N. Sisourat, A. Dubois and J. P. Hansen, *Non perturbative treatment of single ionization of H_2 by fast, highly charged ion impact*, submitted for publication (2009)
13. T. Birkeland, R. Nepstad and M. Førre, *Multiphoton Double Ionization in Helium Driven by Intense XUV Attosecond Pulses*, to be submitted

Scientific Results

1. T. Birkeland, M. Førre, J. P. Hansen and S. Selstø, *Dynamics of H_{2p} ionization in ultrashort strong laser pulses*, J. Phys. B At. Mol. Opt. Phys, **37** 4205-4219 (2004)
2. T. Birkeland and T. Sørevik *Parallel Redistribution of Multidimensional Data* Proceedings ParCo 2007 Conference NIC Series Volume **38**, (2007)
3. V. Popsueva, R. Nepstad, T. Birkeland, M. Førre, J. P. Hansen, E. Lindroth and E. Waltersson, *Structure of lateral two-electron quantum dot molecules in electromagnetic fields* Physical Review B, **76**, 035303 (2007)
4. L. Sælen, I. Sundvor, T. Birkeland, S. Selstø, and M. Førre, *Classical and quantum-mechanical investigation of the role of nondipole effects on the binding of a stripped HD^{2+} molecule* Physical Review A, **76**, 013415 (2007)
5. T. Sørevik, T. Birkeland and G. Okša, *Numerical solution of the 3D time dependent Schrödinger equation in spherical coordinates: Spectral basis and effects of split-operator technique* Journal of Computational and Applied Mathematics, **225**, 56-67 (2007)
6. C. R. Calvert, T. Birkeland, R. B. King, I. D. Williams and J. F. McCann, *Quantum chessboards in the deuterium molecular ion* J. Phys. B: At. Mol. Opt. Phys., **41**, 205504 (2008)
7. T. Birkeland and T. Sørevik, *Parallel Pseudo-spectral Methods for the Time Dependent Schrödinger Equation* Parallel Computing: Numerics, Applications, and Trends R. Trobec, M Vajteršic and P. Zinterhof (ed.) 261-279 (2009)
8. C. R. Calvert, R. B. King, T. Birkeland. J. D. Alexander, J. B. Greenwood, W. A. Bryan, W. R. Newell, D. S. Murphy, J. F. McCann and I. D. Williams, *Pathways to state-selective control of vibrational wavepackets in the deuterium molecular ion* Journal of Modern Optics, **56** 1060-1069 (2009)
9. T. Birkeland and R. Strand, *How to Understand Nano Images*, Techne: Research in Philosophy and Technology, in print (2009)
10. R. Strand and T. Birkeland, *The Science and Politics of Nano Images* Nano meets Macro: Social Perspectives on Nanoscale Sciences and Technologies, (2009)
11. L. Sælen, T. Birkeland, N. Sisourat, A. Dubois and J. P. Hansen, *Full 3D ab initio studies of interference effects in high-energy ion-molecule collisions* Proceedings of ICPEAC XXVI, in print (2009)
12. L. Sælen, T. Birkeland, N. Sisourat, A. Dubois and J. P. Hansen, *Non perturbative treatment of single ionization of H_2 by fast, highly charged ion impact*, submitted for publication (2009)
13. T. Birkeland, R. Nepstad and M. Førre, *Multiphoton Double Ionization in Helium Driven by Intense XUV Attosecond Pulses*, to be submitted

Classical Mechanics

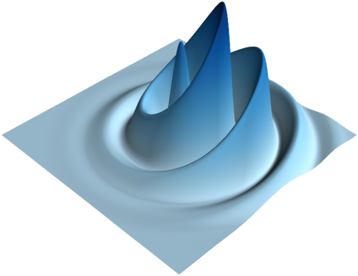


A classical particle has a well defined position and velocity.

The change of velocity is described by Newton's Law

$$\mathbf{F} = m\mathbf{a}$$

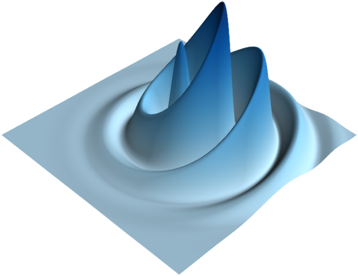
Quantum Mechanics



Heisenberg uncertainty principle: a particle can not have well defined position and velocity

- There is a probability for finding a particle in a given position
- Must therefore consider all possible positions at the same time

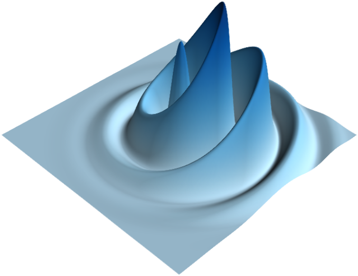
Quantum Mechanics



Heisenberg uncertainty principle: a particle can not have well defined position and velocity

- There is a probability for finding a particle in a given position
- Must therefore consider all possible positions at the same time

Quantum Mechanics



Heisenberg uncertainty principle: a particle can not have well defined position and velocity

- There is a probability for finding a particle in a given position
- Must therefore consider all possible positions at the same time

Mathematical Formulation

Position and velocity is replaced by a *wavefunction*

$$\psi(\mathbf{x}, t)$$

$|\psi(\mathbf{x}, t)|^2$ is the probability density of finding the particle in $\mathbf{x}$

Time evolution of $\psi(\mathbf{x}, t)$ is described by the Time Dependent Schrödinger Equation (TDSE).

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x}, t) = \widehat{H}\psi(\mathbf{x}, t)$$

Mathematical Formulation

Position and velocity is replaced by a *wavefunction*

$$\psi(\mathbf{x}, t)$$

$|\psi(\mathbf{x}, t)|^2$ is the probability density of finding the particle in $\mathbf{x}$

Time evolution of $\psi(\mathbf{x}, t)$ is described by the Time Dependent Schrödinger Equation (TDSE).

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x}, t) = \widehat{H}\psi(\mathbf{x}, t)$$

Hamiltonian

The Hamiltonian describes the energies in the system

$$\widehat{H} = -\frac{1}{2m}\nabla^2 + V(\mathbf{x}, t)$$

- The differentiation operator represents kinetic energy
- $V(\mathbf{x})$ is the potential energy.
- Systems are characterized by different potentials

Hamiltonian

The Hamiltonian describes the energies in the system

$$\widehat{H} = -\frac{1}{2m}\nabla^2 + V(\mathbf{x}, t)$$

- The differentiation operator represents kinetic energy
- $V(\mathbf{x})$ is the potential energy.
- Systems are characterized by different potentials

Hamiltonian

The Hamiltonian describes the energies in the system

$$\widehat{H} = -\frac{1}{2m}\nabla^2 + V(\mathbf{x}, t)$$

- The differentiation operator represents kinetic energy
- $V(\mathbf{x})$ is the potential energy.
- Systems are characterized by different potentials

Hamiltonian

The Hamiltonian describes the energies in the system

$$\widehat{H} = -\frac{1}{2m}\nabla^2 + V(\mathbf{x}, t)$$

- The differentiation operator represents kinetic energy
- $V(\mathbf{x})$ is the potential energy.
- Systems are characterized by different potentials

Adding Particles

- Adding a particle is equivalent to adding degrees of freedom

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x}_1,\mathbf{x}_2,t) = \left(H_1(\mathbf{x}_1) + H_2(\mathbf{x}_2) + H_{1,2}(\mathbf{x}_1,\mathbf{x}_2)\right)\psi(\mathbf{x}_1,\mathbf{x}_2,t)$$

- The time for solving a system increases exponentially with the number of particles
  - 1 particle: 1 sec
  - 2 particles: 17 min
  - 3 particles: 277 hours
  - 7 particles: age of the universe
- The “exponential wall” of quantum mechanics

Adding Particles

- Adding a particle is equivalent to adding degrees of freedom

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x}_1,\mathbf{x}_2,t) = \left(H_1(\mathbf{x}_1) + H_2(\mathbf{x}_2) + H_{1,2}(\mathbf{x}_1,\mathbf{x}_2)\right)\psi(\mathbf{x}_1,\mathbf{x}_2,t)$$

- The time for solving a system increases exponentially with the number of particles
  - 1 particle: 1 sec
  - 2 particles: 17 min
  - 3 particles: 277 hours
  - 7 particles: age of the universe
- The “exponential wall” of quantum mechanics

Adding Particles

- Adding a particle is equivalent to adding degrees of freedom

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x}_1, \mathbf{x}_2, t) = \left(H_1(\mathbf{x}_1) + H_2(\mathbf{x}_2) + H_{1,2}(\mathbf{x}_1, \mathbf{x}_2)\right)\psi(\mathbf{x}_1, \mathbf{x}_2, t)$$

- The time for solving a system increases exponentially with the number of particles
  - 1 particle: 1 sec
  - 2 particles: 17 min
  - 3 particles: 277 hours
  - 7 particles: age of the universe
- The "exponential wall" of quantum mechanics

Adding Particles

- Adding a particle is equivalent to adding degrees of freedom

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x}_1, \mathbf{x}_2, t) = \left(H_1(\mathbf{x}_1) + H_2(\mathbf{x}_2) + H_{1,2}(\mathbf{x}_1, \mathbf{x}_2)\right)\psi(\mathbf{x}_1, \mathbf{x}_2, t)$$

- The time for solving a system increases exponentially with the number of particles
  - 1 particle: 1 sec
  - 2 particles: 17 min
  - 3 particles: 277 hours
  - 7 particles: age of the universe
- The "exponential wall" of quantum mechanics

Adding Particles

- Adding a particle is equivalent to adding degrees of freedom

$$i\frac{\partial}{\partial t}\psi(\mathbf{x}_1, \mathbf{x}_2, t) = \left(H_1(\mathbf{x}_1) + H_2(\mathbf{x}_2) + H_{1,2}(\mathbf{x}_1, \mathbf{x}_2)\right)\psi(\mathbf{x}_1, \mathbf{x}_2, t)$$

- The time for solving a system increases exponentially with the number of particles
  - 1 particle: 1 sec
  - 2 particles: 17 min
  - 3 particles: 277 hours
  - 7 particles: age of the universe
- The "exponential wall" of quantum mechanics

Adding Particles

- Adding a particle is equivalent to adding degrees of freedom

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x}_1,\mathbf{x}_2,t) = \left(H_1(\mathbf{x}_1) + H_2(\mathbf{x}_2) + H_{1,2}(\mathbf{x}_1,\mathbf{x}_2)\right)\psi(\mathbf{x}_1,\mathbf{x}_2,t)$$

- The time for solving a system increases exponentially with the number of particles
  - 1 particle: 1 sec
  - 2 particles: 17 min
  - 3 particles: 277 hours
  - 7 particles: age of the universe
- The “exponential wall” of quantum mechanics

Adding Particles

- Adding a particle is equivalent to adding degrees of freedom

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x}_1, \mathbf{x}_2, t) = \left(H_1(\mathbf{x}_1) + H_2(\mathbf{x}_2) + H_{1,2}(\mathbf{x}_1, \mathbf{x}_2)\right)\psi(\mathbf{x}_1, \mathbf{x}_2, t)$$

- The time for solving a system increases exponentially with the number of particles
  - 1 particle: 1 sec
  - 2 particles: 17 min
  - 3 particles: 277 hours
  - 7 particles: age of the universe
- The "exponential wall" of quantum mechanics

Adding Particles

- Adding a particle is equivalent to adding degrees of freedom

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x}_1, \mathbf{x}_2, t) = \left(H_1(\mathbf{x}_1) + H_2(\mathbf{x}_2) + H_{1,2}(\mathbf{x}_1, \mathbf{x}_2)\right)\psi(\mathbf{x}_1, \mathbf{x}_2, t)$$

- The time for solving a system increases exponentially with the number of particles
  - 1 particle: 1 sec
  - 2 particles: 17 min
  - 3 particles: 277 hours
  - 7 particles: age of the universe
- The "exponential wall" of quantum mechanics

Returning to the TDSE

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \widehat{H}\psi(\mathbf{x},t)$$

Problem: if we know the $\psi(\mathbf{x},t)$, find $\psi(\mathbf{x},t+h)$.

- Can only be solved by hand for the simplest systems
- Computers does not work on continuous problems, the TDSE must therefore be *discretized* in space and time.

Returning to the TDSE

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \widehat{H}\psi(\mathbf{x},t)$$

Problem: if we know the $\psi(\mathbf{x},t)$, find $\psi(\mathbf{x},t+h)$.

- Can only be solved by hand for the simplest systems
- Computers does not work on continuous problems, the TDSE must therefore be *discretized* in space and time.

Returning to the TDSE

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \widehat{H}\psi(\mathbf{x},t)$$

Problem: if we know the $\psi(\mathbf{x},t)$, find $\psi(\mathbf{x},t+h)$.

- Can only be solved by hand for the simplest systems
- Computers does not work on continuous problems, the TDSE must therefore be *discretized* in space and time.

Returning to the TDSE

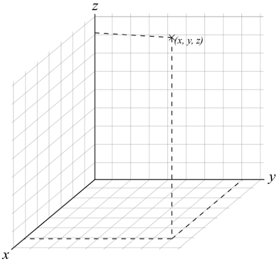
$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \widehat{H}\psi(\mathbf{x},t)$$

Problem: if we know the $\psi(\mathbf{x},t)$, find $\psi(\mathbf{x},t+h)$.

- Can only be solved by hand for the simplest systems
- Computers does not work on continuous problems, the TDSE must therefore be *discretized* in space and time.

Choice of coordinate system

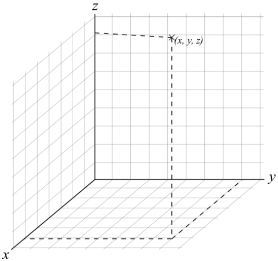
Must choose a coordinate system in which to represent the multi-dimensional wavefunction.



- Cartesian coordinates, $\mathbf{x} = (x, y, z)$
- Spherical coordinates, $\mathbf{x} = (r, \theta, \phi)$
- Cylindrical coordinates, $\mathbf{x} = (r, \rho, \phi)$
- Each rank may be discretized independently
- Optimal choice is system dependent

Choice of coordinate system

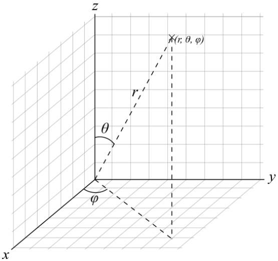
Must choose a coordinate system in which to represent the multi-dimensional wavefunction.



- Cartesian coordinates, $\mathbf{x} = (x, y, z)$
- Spherical coordinates, $\mathbf{x} = (r, \theta, \phi)$
- Cylindrical coordinates, $\mathbf{x} = (r, \rho, \phi)$
- Each rank may be discretized independently
- Optimal choice is system dependent

Choice of coordinate system

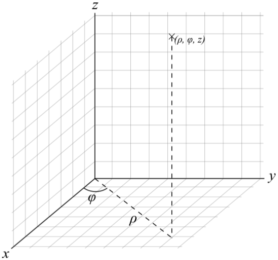
Must choose a coordinate system in which to represent the multi-dimensional wavefunction.



- Cartesian coordinates, $\mathbf{x} = (x, y, z)$
- Spherical coordinates, $\mathbf{x} = (r, \theta, \phi)$
- Cylindrical coordinates, $\mathbf{x} = (r, \rho, \phi)$
- Each rank may be discretized independently
- Optimal choice is system dependent

Choice of coordinate system

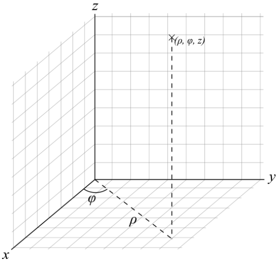
Must choose a coordinate system in which to represent the multi-dimensional wavefunction.



- Cartesian coordinates, $\mathbf{x} = (x, y, z)$
- Spherical coordinates, $\mathbf{x} = (r, \theta, \phi)$
- Cylindrical coordinates, $\mathbf{x} = (r, \rho, \phi)$
- Each rank may be discretized independently
- Optimal choice is system dependent

Choice of coordinate system

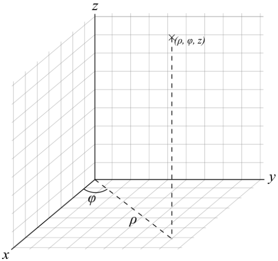
Must choose a coordinate system in which to represent the multi-dimensional wavefunction.



- Cartesian coordinates, $\mathbf{x} = (x, y, z)$
- Spherical coordinates, $\mathbf{x} = (r, \theta, \phi)$
- Cylindrical coordinates, $\mathbf{x} = (r, \rho, \phi)$
- Each rank may be discretized independently
- Optimal choice is system dependent

Choice of coordinate system

Must choose a coordinate system in which to represent the multi-dimensional wavefunction.



- Cartesian coordinates, $\mathbf{x} = (x, y, z)$
- Spherical coordinates, $\mathbf{x} = (r, \theta, \phi)$
- Cylindrical coordinates, $\mathbf{x} = (r, \rho, \phi)$
- Each rank may be discretized independently
- Optimal choice is system dependent

Discretization

- Approximating the continuous problem with a finite number of states.
- Sum of continuous basis functions

$$\psi(x,t) \approx \sum_{i=0}^{m} c_i(t) B_i(x)$$

- Perform calculations on $\mathbf{c}(t) = \{c_i(t)\}$
- Which basis functions should we use?
  - Fourier functions?
  - Orthogonal polynomials?
  - B-Splines?
- Optimal choice is system dependent

Discretization

- Approximating the continuous problem with a finite number of states.
- Sum of continuous basis functions

$$\psi(x,t) \approx \sum_{i=0}^{m} c_i(t) B_i(x)$$

- Perform calculations on $\mathbf{c}(t) = \{c_i(t)\}$
- Which basis functions should we use?
  - Fourier functions?
  - Orthogonal polynomials?
  - B-Splines?
- Optimal choice is system dependent

Discretization

- Approximating the continuous problem with a finite number of states.
- Sum of continuous basis functions

$$\psi(x,t) \approx \sum_{i=0}^{m} c_i(t) B_i(x)$$

- Perform calculations on $\mathbf{c}(t) = \{c_i(t)\}$
- Which basis functions should we use?
  - Fourier functions?
  - Orthogonal polynomials?
  - B-Splines?
- Optimal choice is system dependent

Discretization

- Approximating the continuous problem with a finite number of states.
- Sum of continuous basis functions

$$\psi(x,t) \approx \sum_{i=0}^{m} c_i(t) B_i(x)$$

- Perform calculations on $\mathbf{c}(t) = \{c_i(t)\}$
- Which basis functions should we use?
  - Fourier functions?
  - Orthogonal polynomials?
  - B-Splines?
- Optimal choice is system dependent

Discretization

- Approximating the continuous problem with a finite number of states.
- Sum of continuous basis functions

$$\psi(x,t) \approx \sum_{i=0}^{m} c_i(t) B_i(x)$$

- Perform calculations on $\mathbf{c}(t) = \{c_i(t)\}$
- Which basis functions should we use?
  - Fourier functions?
  - Orthogonal polynomials?
  - B-Splines?
- Optimal choice is system dependent

Propagation

Given a discretization scheme, we can turn the TDSE from

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \widehat{H}\psi(\mathbf{x},t) \quad \rightarrow \quad \mathrm{i}\mathbf{S}\frac{\partial}{\partial t}\mathbf{c}(t) = \mathbf{H}\mathbf{c}(t)$$

- Propagation: from $\mathbf{c}(t)$, find $\mathbf{c}(t+h)$
- Choice of propagation scheme
  - Cayley Propagator
  - Split-Step Propagator
  - Krylov Propagator
- Can be done independently from space discretization
- Optimal propagation scheme is system dependent

Propagation

Given a discretization scheme, we can turn the TDSE from

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \widehat{H}\psi(\mathbf{x},t) \quad \rightarrow \quad \mathrm{i}\mathbf{S}\frac{\partial}{\partial t}\mathbf{c}(t) = \mathbf{H}\mathbf{c}(t)$$

- Propagation: from $\mathbf{c}(t)$, find $\mathbf{c}(t+h)$
- Choice of propagation scheme
  - Cayley Propagator
  - Split-Step Propagator
  - Krylov Propagator
- Can be done independently from space discretization
- Optimal propagation scheme is system dependent

Propagation

Given a discretization scheme, we can turn the TDSE from

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \widehat{H}\psi(\mathbf{x},t) \quad \rightarrow \quad \mathrm{i}\mathbf{S}\frac{\partial}{\partial t}\mathbf{c}(t) = \mathbf{H}\mathbf{c}(t)$$

- Propagation: from $\mathbf{c}(t)$, find $\mathbf{c}(t+h)$
- Choice of propagation scheme
  - Cayley Propagator
  - Split-Step Propagator
  - Krylov Propagator
- Can be done independently from space discretization
- Optimal propagation scheme is system dependent

Propagation

Given a discretization scheme, we can turn the TDSE from

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \widehat{H}\psi(\mathbf{x},t) \quad \rightarrow \quad \mathrm{i}\mathbf{S}\frac{\partial}{\partial t}\mathbf{c}(t) = \mathbf{H}\mathbf{c}(t)$$

- Propagation: from $\mathbf{c}(t)$, find $\mathbf{c}(t+h)$
- Choice of propagation scheme
  - Cayley Propagator
  - Split-Step Propagator
  - Krylov Propagator
- Can be done independently from space discretization
- Optimal propagation scheme is system dependent

Propagation

Given a discretization scheme, we can turn the TDSE from

$$\mathrm{i}\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \widehat{H}\psi(\mathbf{x},t) \quad \rightarrow \quad \mathrm{i}\mathbf{S}\frac{\partial}{\partial t}\mathbf{c}(t) = \mathbf{H}\mathbf{c}(t)$$

- Propagation: from $\mathbf{c}(t)$, find $\mathbf{c}(t+h)$
- Choice of propagation scheme
  - Cayley Propagator
  - Split-Step Propagator
  - Krylov Propagator
- Can be done independently from space discretization
- Optimal propagation scheme is system dependent

Solving the TDSE - Summary

- System dependent choices
  - coordinate system
  - discretization scheme
  - propagator
- Making the right choice is difficult
- The wrong choice can lead to hard-to-solve systems
- A flexible solver should allow experimentation with different methods

Solving the TDSE - Summary

- System dependent choices
  - coordinate system
  - discretization scheme
  - propagator
- Making the right choice is difficult
- The wrong choice can lead to hard-to-solve systems
- A flexible solver should allow experimentation with different methods

Solving the TDSE - Summary

- System dependent choices
  - coordinate system
  - discretization scheme
  - propagator
- Making the right choice is difficult
- The wrong choice can lead to hard-to-solve systems
- A flexible solver should allow experimentation with different methods

Solving the TDSE - Summary

- System dependent choices
  - coordinate system
  - discretization scheme
  - propagator
- Making the right choice is difficult
- The wrong choice can lead to hard-to-solve systems
- A flexible solver should allow experimentation with different methods

PyProp Framework Design

- Core Routines
- Independent Modules
- User Code

PyProp Framework Design

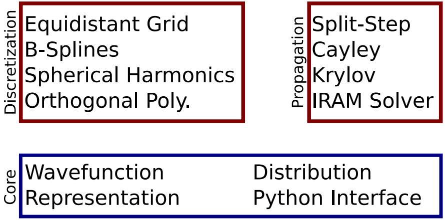
- Core Routines
- Independent Modules
- User Code

Core

Wavefunction	Distribution
Representation	Python Interface

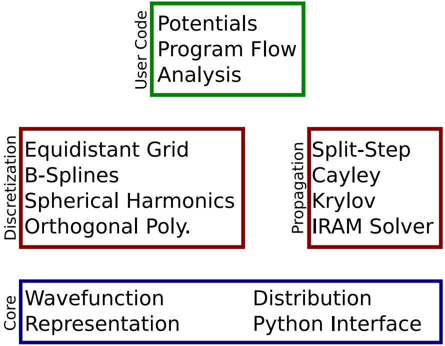
PyProp Framework Design

- Core Routines
- Independent Modules
- User Code



PyProp Framework Design

- Core Routines
- Independent Modules
- User Code



Flexibility

- Choose dimensionality and discretization
  - Several discretization schemes built in
  - Can calculate inner products, operator-wavefunction multiplications, load/save wavefunctions
- Supply potentials
  - PyProp takes care of a lot of repetetive code
- Choose propagator
  - Several propagators built in
- Perform analysis and data exploration
  - High level code is written in Python
  - All the propagation tools can be used interactively

Flexibility

- Choose dimensionality and discretization
  - Several discretization schemes built in
  - Can calculate inner products, operator-wavefunction multiplications, load/save wavefunctions
- Supply potentials
  - PyProp takes care of a lot of repetetive code
- Choose propagator
  - Several propagators built in
- Perform analysis and data exploration
  - High level code is written in Python
  - All the propagation tools can be used interactively

Flexibility

- Choose dimensionality and discretization
  - Several discretization schemes built in
  - Can calculate inner products, operator-wavefunction multiplications, load/save wavefunctions
- Supply potentials
  - PyProp takes care of a lot of repetetive code
- Choose propagator
  - Several propagators built in
- Perform analysis and data exploration
  - High level code is written in Python
  - All the propagation tools can be used interactively

Flexibility

- Choose dimensionality and discretization
  - Several discretization schemes built in
  - Can calculate inner products, operator-wavefunction multiplications, load/save wavefunctions
- Supply potentials
  - PyProp takes care of a lot of repetetive code
- Choose propagator
  - Several propagators built in
- Perform analysis and data exploration
  - High level code is written in Python
  - All the propagation tools can be used interactively

Performance

- Practical calculations can have wavefunctions with $1\,\mathrm{B}$ elements.
- Computational kernels are optimized
  - Using high performance libraries where possible
  - Written in C++/Fortran
- Automatic parallelization of one or more ranks
  - Supports redistribution
  - Parallel matrix-vector operations

Performance

- Practical calculations can have wavefunctions with $1\,\mathrm{B}$ elements.
- Computational kernels are optimized
  - Using high performance libraries where possible
  - Written in C++/Fortran
- Automatic parallelization of one or more ranks
  - Supports redistribution
  - Parallel matrix-vector operations

Performance

- Practical calculations can have wavefunctions with $1\,\mathrm{B}$ elements.
- Computational kernels are optimized
  - Using high performance libraries where possible
  - Written in C++/Fortran
- Automatic parallelization of one or more ranks
  - Supports redistribution
  - Parallel matrix-vector operations

Current Applications

Numerics:

- Generalized reduced wavefunctions (Lundeland and Kozlov)
- Multidimensional Redistribution (ParCo 2007 p443 (2008))
- Trans. Chebyshev Grids (J. Comp. Appl. Math. 225 p56 (2009))

Physics:

- Two Electron Quantum Dots (Phys. Rev. B 76, 035303 (2007))
- Laser-bound Molecules (Phys. Rev. A 76, 013415 (2007))
- Vibrational Molecular Wavepackets (J. Phys. B 41 205504 (2008))
- Laser Ionization of SAE Argon (Nepstad et.al. (2009))
- Ion-Molecule Collsion (Submitted)
- Laser Ionization of Two-Electron Helium (In preparation)
- Laser Ionization of H_2 (work in progress)
- Born-Oppenheimer effects in H_2^+ (work in progress)

Current Applications

Numerics:

- Generalized reduced wavefunctions (Lundeland and Kozlov)
- Multidimensional Redistribution (ParCo 2007 p443 (2008))
- Trans. Chebyshev Grids (J. Comp. Appl. Math. 225 p56 (2009))

Physics:

- Two Electron Quantum Dots (Phys. Rev. B 76, 035303 (2007))
- Laser-bound Molecules (Phys. Rev. A 76, 013415 (2007))
- Vibrational Molecular Wavepackets (J. Phys. B 41 205504 (2008))
- Laser Ionization of SAE Argon (Nepstad et.al. (2009))
- Ion-Molecule Collsion (Submitted)
- Laser Ionization of Two-Electron Helium (In preparation)
- Laser Ionization of H_2 (work in progress)
- Born-Oppenheimer effects in H_2^+ (work in progress)

Current Applications

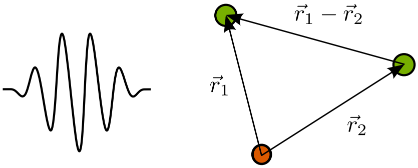
Numerics:

- Generalized reduced wavefunctions (Lundeland and Kozlov)
- Multidimensional Redistribution (ParCo 2007 p443 (2008))
- Trans. Chebyshev Grids (J. Comp. Appl. Math. 225 p56 (2009))

Physics:

- Two Electron Quantum Dots (Phys. Rev. B 76, 035303 (2007))
- Laser-bound Molecules (Phys. Rev. A 76, 013415 (2007))
- Vibrational Molecular Wavepackets (J. Phys. B 41 205504 (2008))
- Laser Ionization of SAE Argon (Nepstad et.al. (2009))
- Ion-Molecule Collsion (Submitted)
- Laser Ionization of Two-Electron Helium (In preparation)
- Laser Ionization of H_2 (work in progress)
- Born-Oppenheimer effects in H_2^+ (work in progress)

Example: Laser Ionization of Helium



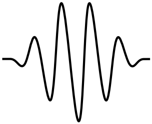
- Two electron system

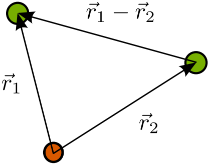
$$\widehat{H}_0(\mathbf{r}_i) = -\frac{1}{2}\nabla^2 - \frac{2}{r_i} + A_z(t)\left(\frac{\partial}{\partial z_i} - \frac{\cos\theta_i}{r_i}\right)$$

$$\widehat{H}(\mathbf{r}_1, \mathbf{r}_2) = \widehat{H}_0(\mathbf{r}_1) + \widehat{H}_0(\mathbf{r}_2) + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

- Near spherical symmetry around the nucleus

Example: Laser Ionization of Helium



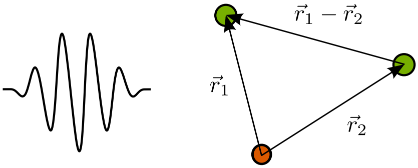


- Two electron system

$$\widehat{H}_0(\mathbf{r}_i) = -\frac{1}{2}\nabla^2 - \frac{2}{r_i} + A_z(t)\left(\frac{\partial}{\partial z_i} - \frac{\cos\theta_i}{r_i}\right)$$

$$\widehat{H}(\mathbf{r}_1, \mathbf{r}_2) = \widehat{H}_0(\mathbf{r}_1) + \widehat{H}_0(\mathbf{r}_2) + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

- Near spherical symmetry around the nucleus



- Two electron system

$$\widehat{H}_0(\mathbf{r}_i) = -\frac{1}{2}\nabla^2 - \frac{2}{r_i} + A_z(t)\left(\frac{\partial}{\partial z_i} - \frac{\cos\theta_i}{r_i}\right)$$

$$\widehat{H}(\mathbf{r}_1, \mathbf{r}_2) = \widehat{H}_0(\mathbf{r}_1) + \widehat{H}_0(\mathbf{r}_2) + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

- Near spherical symmetry around the nucleus

Helium in PyProp

- Three computational ranks
  1. $\mathcal{Y}^{L,M}_{l_1,l_2}(\Omega_1,\Omega_2)$ - Combination of all angles
  2. r_1 - distance from nucleus to first electron
  3. r_2 - distance from nucleus to second electron
- Discretizing r_1 and r_2 with B-Splines
- Total wavefunction has $\approx 10\,\mathrm{M}$ elements
  - Total memory requirement is $\approx 100\,\mathrm{GB}$
  - Must be run in parallel
- Propagation with the Cayley Propagator
- A calculation typically takes $24\,\mathrm{h}$ on $111\,\mathrm{CPUs}$

Helium in PyProp

- Three computational ranks
  1. $\mathcal{Y}_{l_1,l_2}^{L,M}(\Omega_1, \Omega_2)$ - Combination of all angles
  2. r_1 - distance from nucleus to first electron
  3. r_2 - distance from nucleus to second electron
- Discretizing r_1 and r_2 with B-Splines
- Total wavefunction has $\approx 10\,\mathrm{M}$ elements
  - Total memory requirement is $\approx 100\,\mathrm{GB}$
  - Must be run in parallel
- Propagation with the Cayley Propagator
- A calculation typically takes $24\,\mathrm{h}$ on $111\,\mathrm{CPUs}$

Helium in PyProp

- Three computational ranks
  1. $\mathcal{Y}^{L,M}_{l_1,l_2}(\Omega_1,\Omega_2)$ - Combination of all angles
  2. r_1 - distance from nucleus to first electron
  3. r_2 - distance from nucleus to second electron
- Discretizing r_1 and r_2 with B-Splines
- Total wavefunction has $\approx 10\,\mathrm{M}$ elements
  - Total memory requirement is $\approx 100\,\mathrm{GB}$
  - Must be run in parallel
- Propagation with the Cayley Propagator
- A calculation typically takes $24\,\mathrm{h}$ on $111\,\mathrm{CPUs}$

Helium in PyProp

- Three computational ranks
  1. $\mathcal{Y}_{l_1,l_2}^{L,M}(\Omega_1, \Omega_2)$ - Combination of all angles
  2. r_1 - distance from nucleus to first electron
  3. r_2 - distance from nucleus to second electron
- Discretizing r_1 and r_2 with B-Splines
- Total wavefunction has $\approx 10\,\mathrm{M}$ elements
  - Total memory requirement is $\approx 100\,\mathrm{GB}$
  - Must be run in parallel
- Propagation with the Cayley Propagator
- A calculation typically takes $24\,\mathrm{h}$ on $111\,\mathrm{CPUs}$

Helium in PyProp

- Three computational ranks
  1. $\mathcal{Y}_{l_1,l_2}^{L,M}(\Omega_1, \Omega_2)$ - Combination of all angles
  2. r_1 - distance from nucleus to first electron
  3. r_2 - distance from nucleus to second electron
- Discretizing r_1 and r_2 with B-Splines
- Total wavefunction has $\approx 10\,\mathrm{M}$ elements
  - Total memory requirement is $\approx 100\,\mathrm{GB}$
  - Must be run in parallel
- Propagation with the Cayley Propagator
- A calculation typically takes $24\,\mathrm{h}$ on $111\,\mathrm{CPUs}$

Helium - Analysis

- Determine physical quantities
  - Ionization probability
  - Energy distribution
- Remove bound states
  - Use integrated eigenvalue solver
- Project wavefunction on single electron states
  - Use the same discretization and propagation schemes for single electron problems

Helium - Analysis

- Determine physical quantities
  - Ionization probability
  - Energy distribution
- Remove bound states
  - Use integrated eigenvalue solver
- Project wavefunction on single electron states
  - Use the same discretization and propagation schemes for single electron problems

Helium - Analysis

- Determine physical quantities
  - Ionization probability
  - Energy distribution
- Remove bound states
  - Use integrated eigenvalue solver
- Project wavefunction on single electron states
  - Use the same discretization and propagation schemes for single electron problems

Helium - Analysis

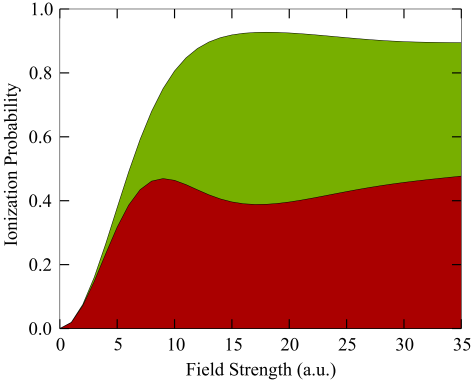
- Determine physical quantities
  - Ionization probability
  - Energy distribution
- Remove bound states
  - Use integrated eigenvalue solver
- Project wavefunction on single electron states
  - Use the same discretization and propagation schemes for single electron problems

Helium - Movie

Animation of an ionization event

Helium - Ionzation Probability

Ionization probability as a function of field strength



- Ionization probability does not go to one (stabilization)
- Each point on the graph is from one ionization event
  - Total of 30000 CPU hours

Summary

- Created a software framework for atomic physics
  - Scalable - can perform massive calculations on large 2 electron systems
  - Flexible - can combine many different discretizations and propagators to solve quite diverse problems
- Solved a variety of problems using PyProp

Summary

- Created a software framework for atomic physics
  - Scalable - can perform massive calculations on large 2 electron systems
  - Flexible - can combine many different discretizations and propagators to solve quite diverse problems
- Solved a variety of problems using PyProp

Summary

- Created a software framework for atomic physics
  - Scalable - can perform massive calculations on large 2 electron systems
  - Flexible - can combine many different discretizations and propagators to solve quite diverse problems
- Solved a variety of problems using PyProp

Summary

- Created a software framework for atomic physics
  - Scalable - can perform massive calculations on large 2 electron systems
  - Flexible - can combine many different discretizations and propagators to solve quite diverse problems
- Solved a variety of problems using PyProp

Future plans

- Ease transition for new users
  - Documentation
  - Simplify installation procedure
  - Better error handling
- Compare methods
- Simplify implementation of new methods

Future plans

- Ease transition for new users
  - Documentation
  - Simplify installation procedure
  - Better error handling
- Compare methods
- Simplify implementation of new methods

Future plans

- Ease transition for new users
  - Documentation
  - Simplify installation procedure
  - Better error handling
- Compare methods
- Simplify implementation of new methods

Future plans

- Ease transition for new users
  - Documentation
  - Simplify installation procedure
  - Better error handling
- Compare methods
- Simplify implementation of new methods

Future plans

- Ease transition for new users
  - Documentation
  - Simplify installation procedure
  - Better error handling
- Compare methods
- Simplify implementation of new methods

Future plans

- Ease transition for new users
  - Documentation
  - Simplify installation procedure
  - Better error handling
- Compare methods
- Simplify implementation of new methods

Image Sources

Wikimedia Commons

- Vitruvian man - File:Vitruvian.jpg
- Hair - File:Human_Hair_40x.JPG
- Cell - File:SEM_blood_cells.jpg
- HIV - File:HIV-budding-Color.jpg
- Atom - File:Stylised_Lithium_Atom.svg

Raymond Nepstad

- Wavefunction
- Helium animation