herramientas de HPC para física de colisiones y reacciones químicas

herramientas de HPC para física de colisiones y reacciones químicas

$$A + BC \longrightarrow A + B + C$$

$$A + BC \longrightarrow A + B + C$$

$$e + H \longrightarrow e + H^{+} + e \text{ ionización}$$

$$A + BC \longrightarrow A + B + C$$

$$e + H \longrightarrow e + H^{+} + e$$

$$H^{+} + H \longrightarrow H^{+} + H^{+} + e \quad \text{ionización}$$

$$A + BC \longrightarrow A + B + C$$

$$e + H \longrightarrow e + H^{+} + e$$

$$H^{+} + H \longrightarrow H^{+} + H^{+} + e$$

$$Li + Li_2 \longrightarrow Li + Li + Li$$

disociación inducida por colisión

$$A + BC \longrightarrow A + B + C$$

$$e + H \longrightarrow e + H^{+} + e$$

$$H^{+} + H \longrightarrow H^{+} + H^{+} + e$$

$$Li + Li_2 \longrightarrow Li + Li + Li$$

$$h\nu + He \longrightarrow e + He^{++} + e$$

Doble Fotoionización

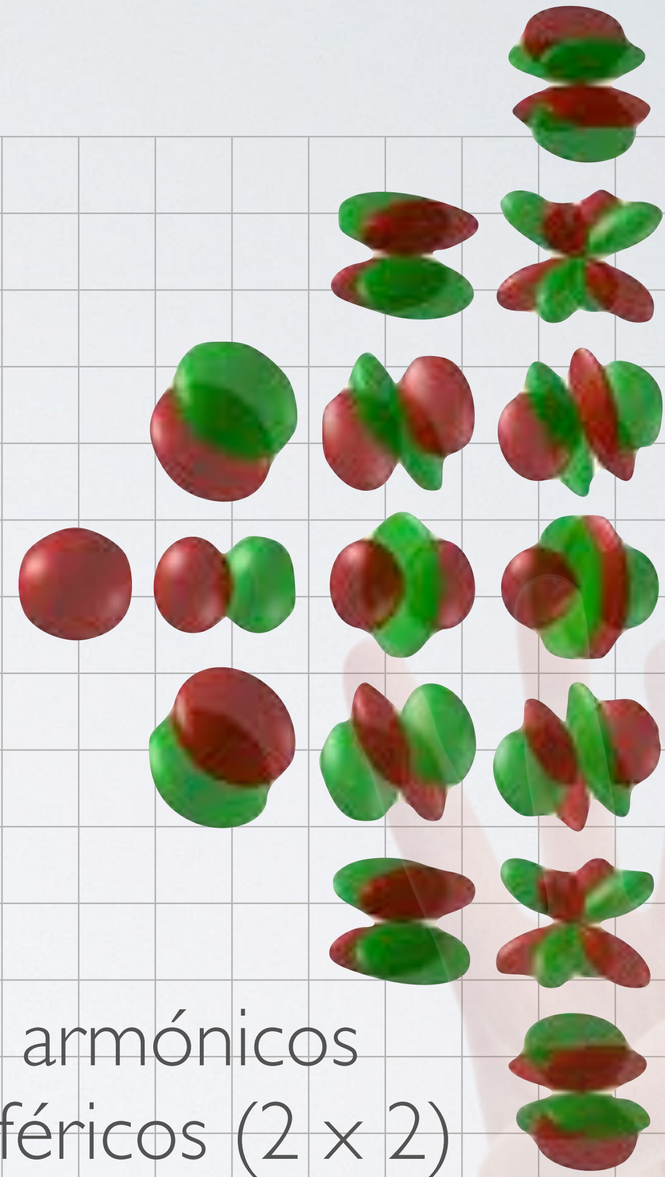
problema de 3 cuerpos cuántico

ecuación de
schrödinger
independiente del tiempo

3 cuerpos x 3 coord. c/u - 3 coord. CM = 6 coord

esféricas

coordenadas esféricas (2 x 3)



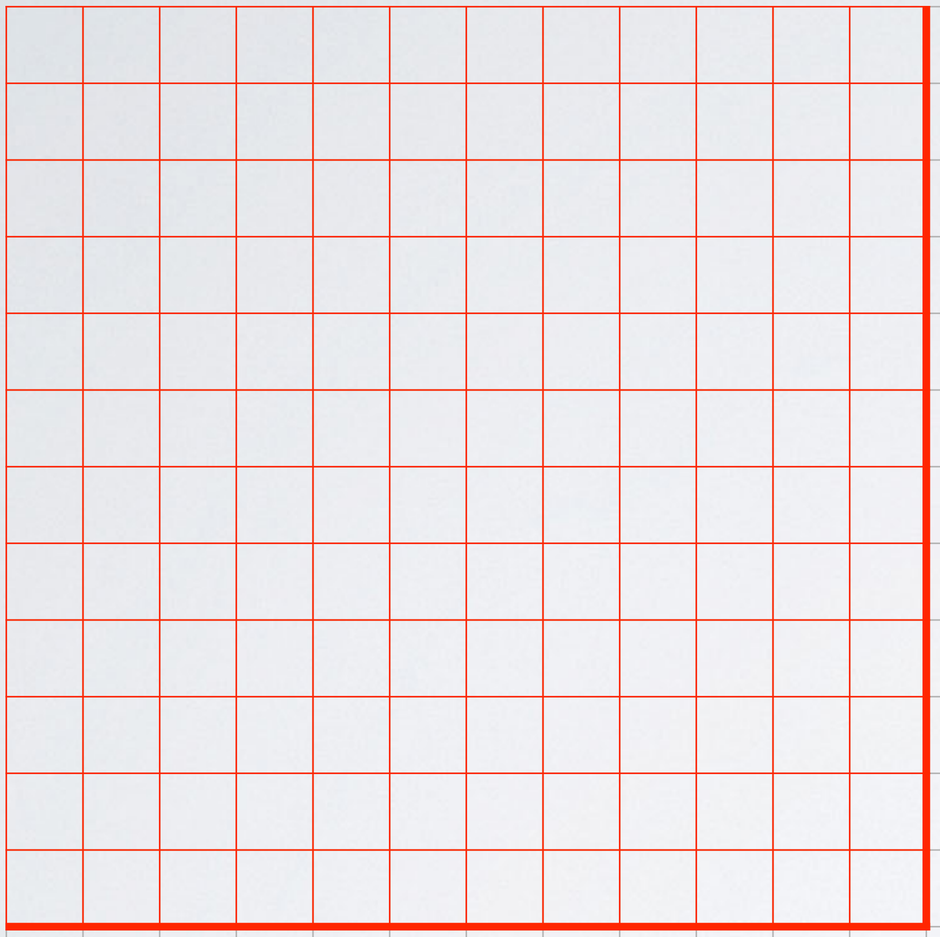
armónicos
esféricos (2 x 2)

dominio radial infinito (2D)

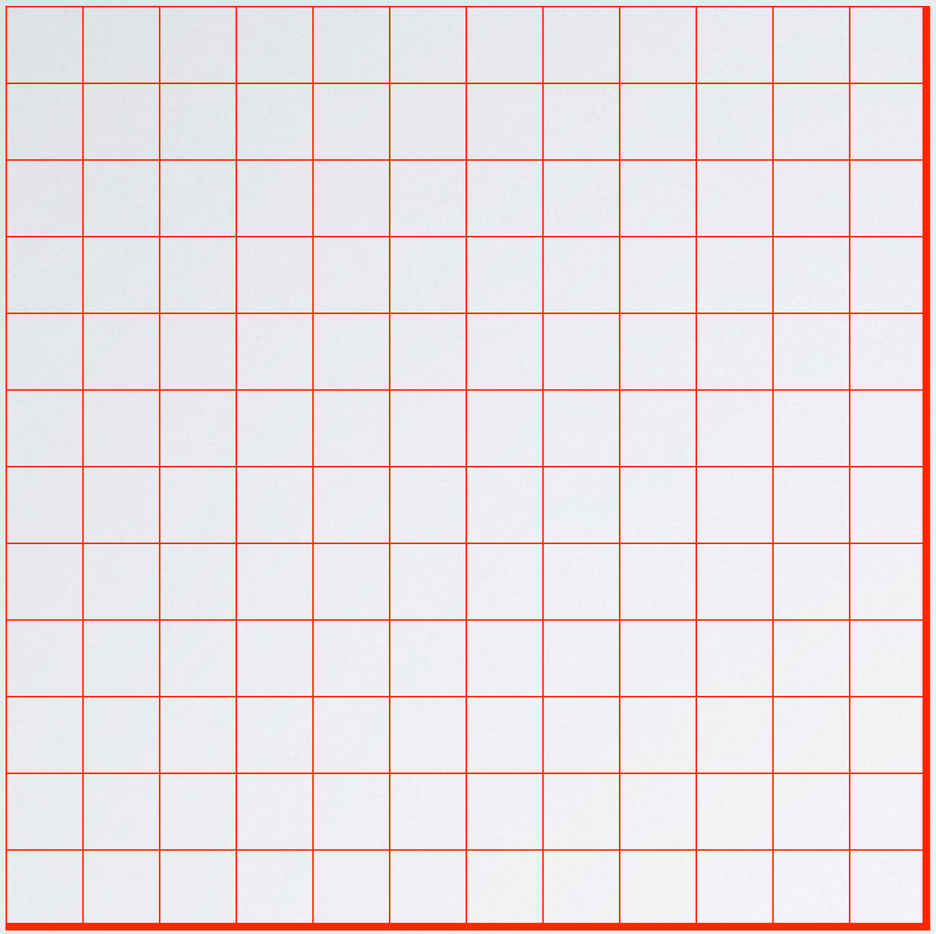
coordenadas esféricas radiales (x2)

dominio radial infinito (2D)

funciones sturmianas generalizadas

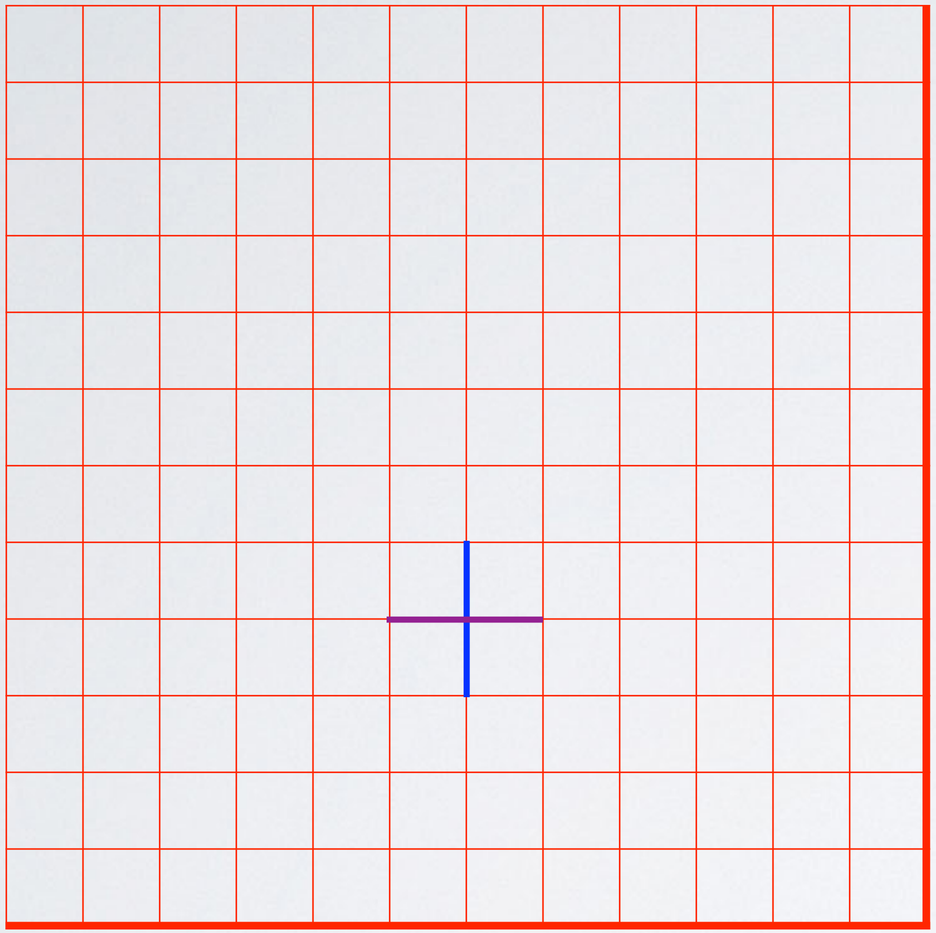


dominio radial **finito** (2D)+ C. C.



dominio radial finito (2D) + C. C.

ecuación
diferencial de
segundo orden en
derivadas parciales con
condiciones de
contorno complejas

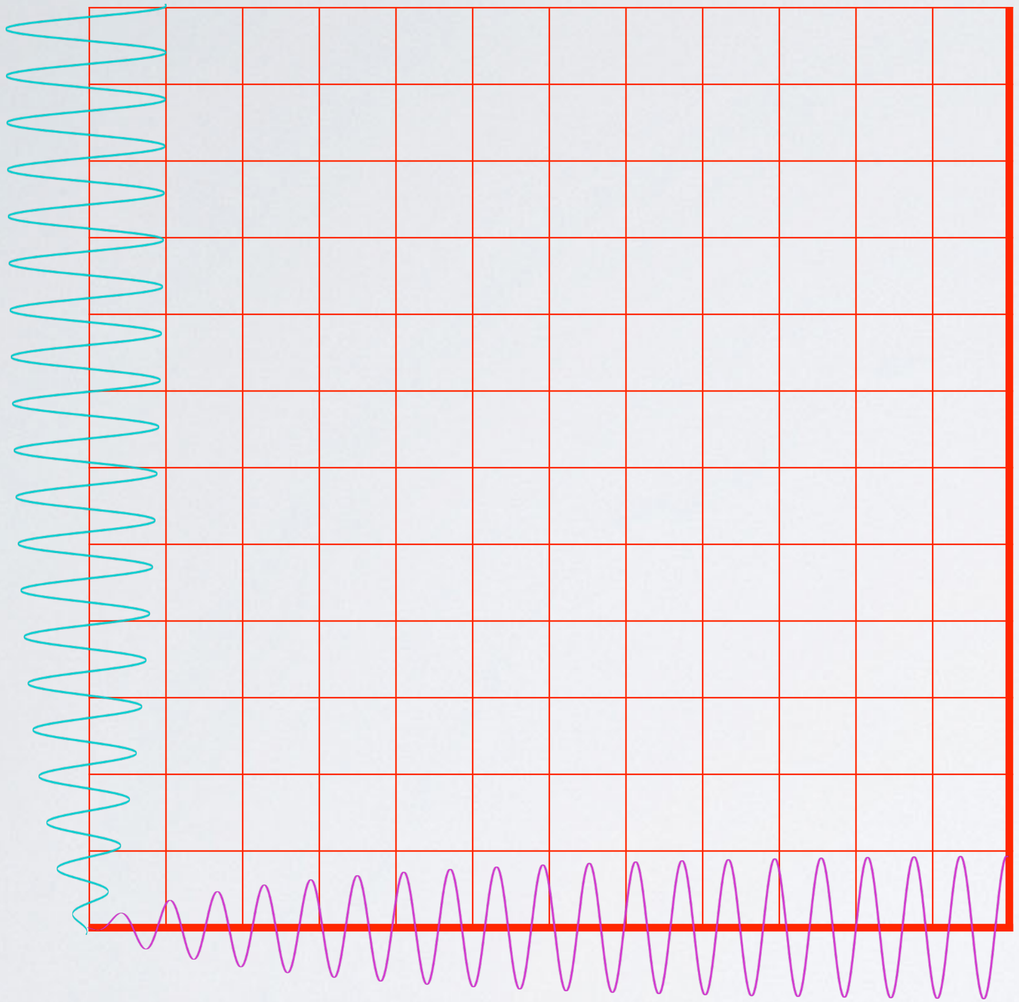


dominio radial finito (2D) + C. C.

discretización en
diferencias finitas

cálculo de la
matriz H

problema de álgebra
lineal numérica
ralo



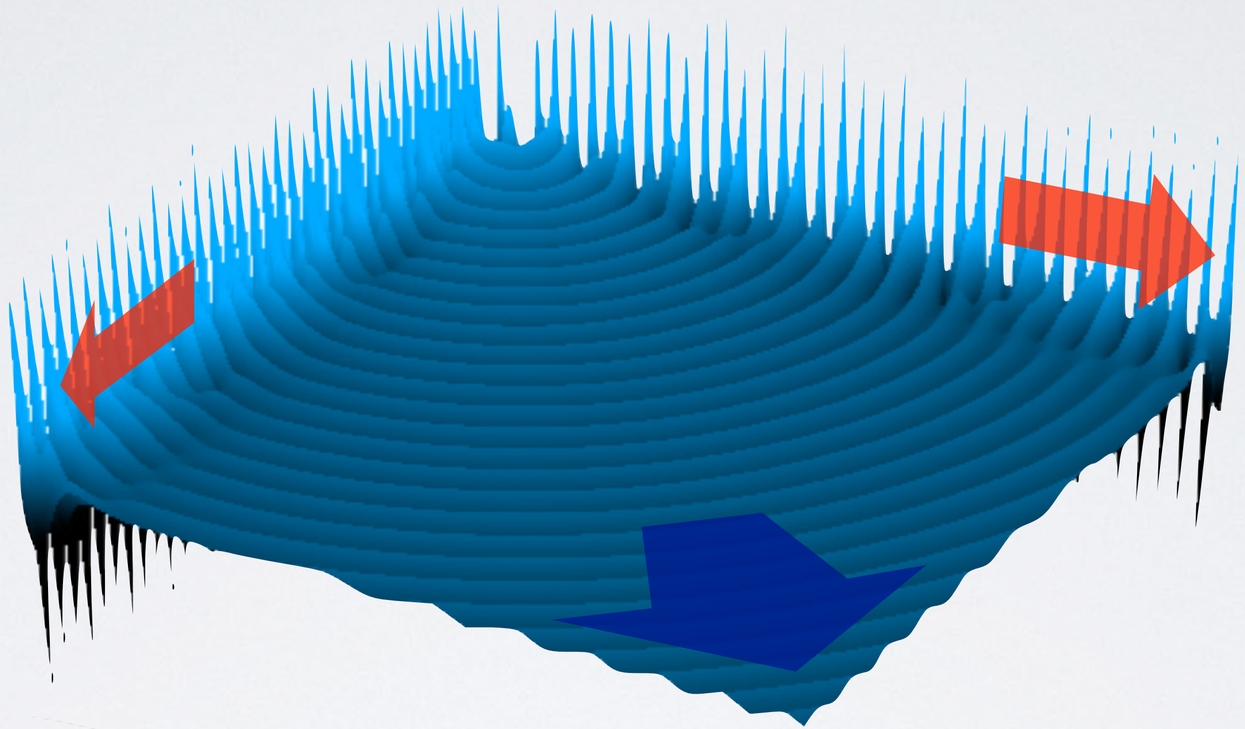
dominio radial finito (2D) + C. C.

método espectral
con funciones sturmianas

cálculo de la
matriz H

problema de álgebra
lineal numérica
denso

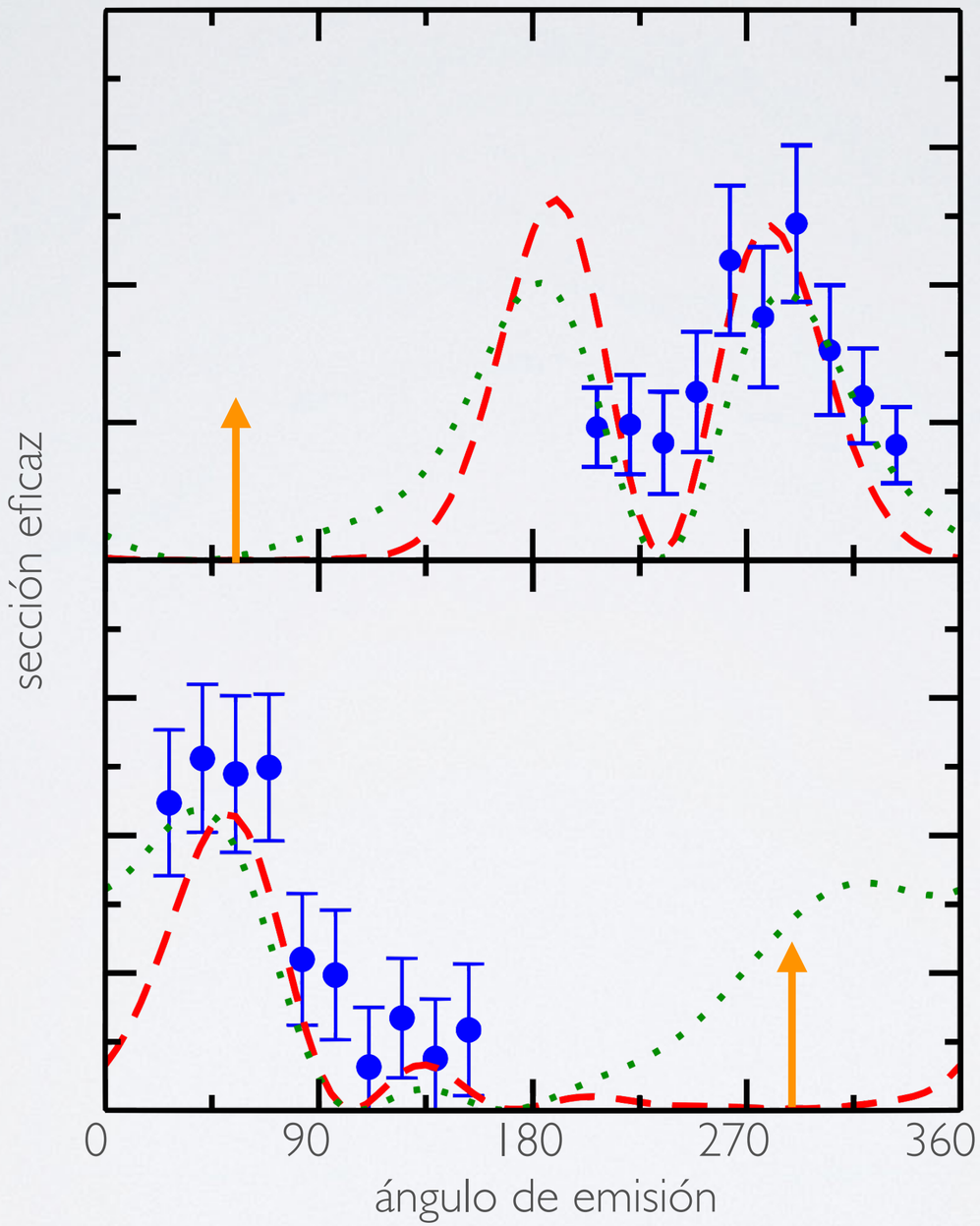
(e,3e) alta energía



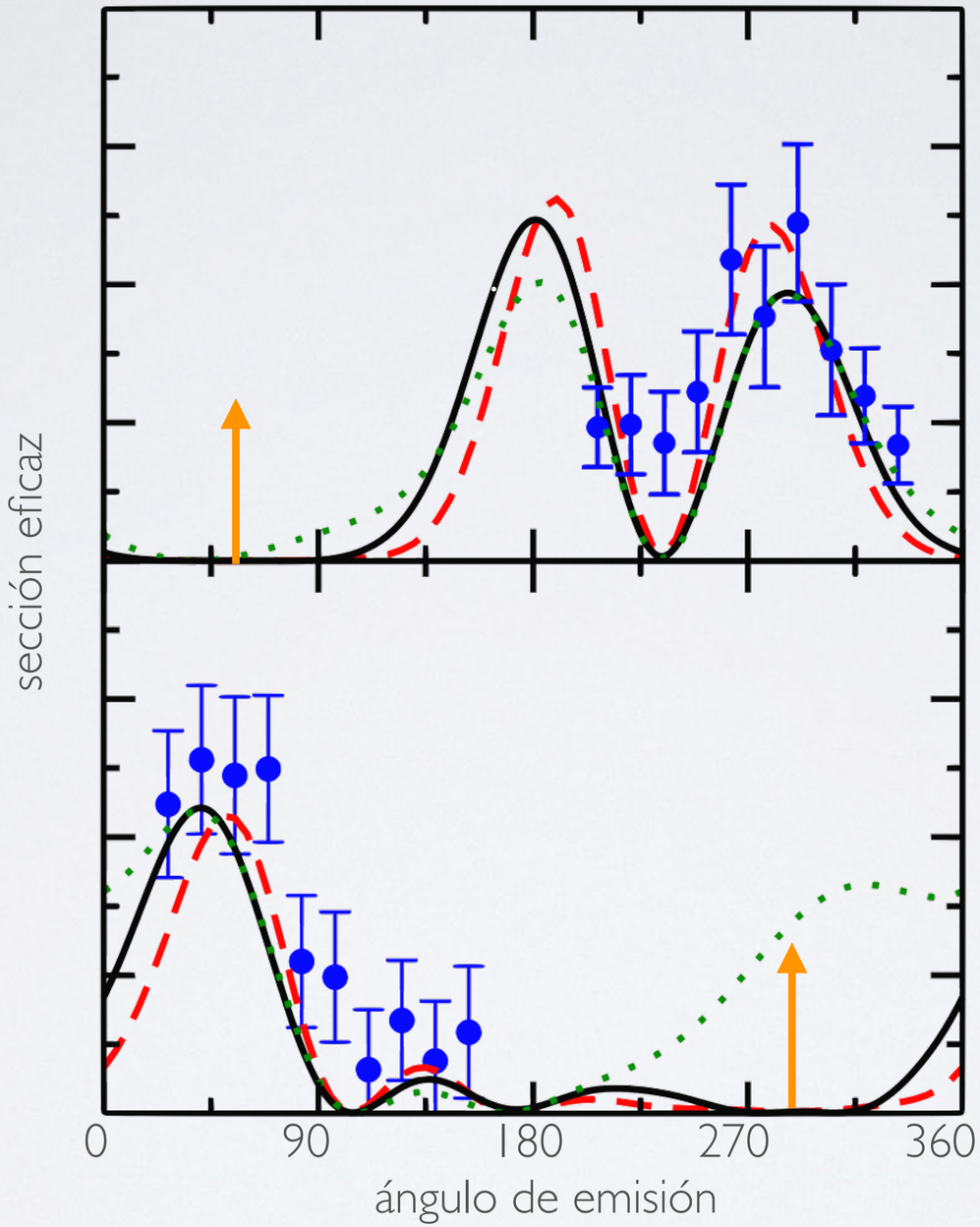
ionización simple
ionización - excitación

doble ionización

(e,3e) alta energía



(e,3e) alta energía



m. ambrosio et al, enviado, 2014

Institute of Physics Publishing — Journal of Physics A: Mathematical and General
J. Phys. A: Math. Gen. 36 (2003) 8443–8462 — PII: S0305-4470(03)62313-9

Two-body Coulomb wavefunctions as kernel for alternative integral transformations

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Abstract
In this paper we investigate different representations of an arbitrary function in terms of two-body Coulomb eigenfunctions. We discuss the standard energy basis in spherical and parabolic coordinates with the purpose of remarking explicitly that two additional parameters appear both in the Schrödinger equation and in the wavefunctions: the charge and the angular momentum. We introduce the charge and generalized angular momentum Sturmian function representations, which result when the charge or the angular momentum is used as the eigenvalue in the Coulomb Schrödinger equation, respectively. We present the connection between the generalized angular momentum representation and the Kontorovich–Lebedev transform. Finally, we extend the angular momentum representation to six dimensions, which is suitable for further applications in the three-body Coulomb problem.

PACS number: 03.65.−w

1. Introduction

The standard way of theoretically studying the properties of a wide variety of atomic and molecular systems is by using functional basis set for representing the physical magnitudes involved in the phenomena under analysis. According to the mathematical structure of quantum mechanics, each physical magnitude has a Hermitian operator associated and then its eigenfunctions become the natural basis set to be used. The most common basis set uses the *energy eigenfunctions*, i.e., the eigenfunctions of the Hamiltonian. However, in some cases the energy eigenfunctions are not the most convenient ones and alternative basis sets are necessary.

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L^2 Discretization of Sturmian Wave Functions for Coulomb-like Potentials

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DOI 10.1002/qua.21220

ABSTRACT: In this work we introduce a method to construct Sturmian functions for general interaction potentials in two-body problems. We expand these Sturmians on a finite L^2 space, using N Laguerre basis functions to obtain a discrete set of eigenvalues for positive and negative energies. Orthogonality and closure relations are thus rewritten for these expansions; completeness is achieved through increasing the basis size. We apply the method to the Coulomb and Herman and Skillman potential. We study the behavior of the functions obtained and their convergence for an overall range of energies. The Sturmian functions are applied to solve the Schrödinger equation for an active electron in a He-like system. © 2006 Wiley Periodicals, Inc. Int J Quantum Chem 107: 832–844, 2007

Key words: Sturmian functions; Coulomb potential; Coulomb screened potential; Pollaczek polynomials

1. Introduction

The theoretical study of a wide range of atomic and molecular properties can be carried out through the representation of a particular physical magnitude by a functional basis set. Such functions are usually generated by solving the Schrödinger equation for the problem under study, or an approximated problem similar to the one of interest. The eigenfunctions obtained are those associated to the energy eigenvalues. However, in some cases, these functions are not suitable to a given problem and other basis sets are necessary or more convenient, e.g., for convergency reasons. As an alternative to energy eigenfunctions one could find solutions to the same wave equation treating the energy as a fixed

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Contract grant sponsor: CONICET.
Contract grant number: PIP 5595.

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CHAPTER SEVEN

Three-Body Coulomb Problems with Generalized Sturmian Functions

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Contents

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153

Discrete Sets of Many-Body Sturmians

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ABSTRACT: In this work, we present a method to obtain two-particle Coulomb Sturmians Functions (CSF) with an expansion in a set of L^2 basis functions. In the two-body case, we recover the exact (discrete) spectrum of the CSFs for negative energies and a discretized approximation for positive ones. Besides, we make use of this method to analyze the two-independent electron problem as a Generalized Sturmian problem. We propose a discretized version of the wave function in terms of the CSF states, and show that the problem reduces to find numerical coincidences between energy-dependent eigencharges of the mutually independent one-electron systems. This expansion methodology includes the continuum information which is lost in the sets used previously in the literature, and is complete when the size of the basis goes to infinity. © 2008 Wiley Periodicals, Inc. Int J Quantum Chem 109: 125–134, 2009

Key words: Sturmians functions; generalized Sturmians; two-electron atoms

1. Introduction

The configuration interaction (CI) method has been widely used to deal with two-electron atomic bound states. Roughly, it is based on the expansion of the wave function in a set of eigenstates of the total angular momentum operator $\mathbf{L}^2$, where the positions of the electrons are determined by the spherical coordinates which locate the electrons relative to the nucleus. By means of such expansion, one arrives to a two-dimensional equation in the radial electronic coordinates, whose solution is approximated as a superposition of two-electron configurations. Other methods in which the basis expands the behavior of the wave function in all the interparticle distances are more rapidly convergent (see [1, 2] and references therein), but generally the calculation is very time consuming, and the algebra is too much complicated to be extended from two to many-electron atoms, compared to the case of the CI scheme.

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Contract grant number: PGI 24/038.

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A General Method to Obtain Sturmian Functions for Continuum and Bound State Problems With Coulomb Interactions

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ABSTRACT: In this article, we investigate discretization schemes to represent Sturmian functions for both positive and negative energies in the presence of a long range Coulomb potential. We explore two methods to obtain Sturmian functions for positive energy. The first one involves the expansion of the radial wave function in a L^2 finite basis set, whereas the second one introduces the discretization of the radial coordinate domain of the Hamiltonian or, alternatively, the Green function. We apply them to find the bound states and scattering phase shift for $\mathcal{N}$-electron atoms close to the critical charge. Both methods are able to describe bound states near threshold, as well as continuum states with very good convergence properties. © 2009 Wiley Periodicals, Inc. Int J Quantum Chem 110: 963–974, 2010

Key words: Sturmian function; scattering; phase shift; critical charge

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Contract grant sponsor: Universidad Nacional del Sur (Argentina).
Contract grant number: PGI 24/F038.
Contract grant sponsor: CONICET (Argentina).
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Accelerating spectral atomic and molecular collisions methods with graphics processing units

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Spectral methods
Sturmian functions
GPU computing

ABSTRACT
We present a computation method to accelerate the calculation of the Hamiltonian of a three-body time independent Schrödinger equation for collisions. The Hamiltonian is constructed with one dimensional (basis overlaps) and two dimensional (interparticle interaction) integrals that are mapped into a computational grid in a Graphics Processing Unit (GPU). We illustrate the method for the case of an electron impact single ionization of a two electron atom. This proposal makes use of a Generalized Sturmian Basis set for each electron, which are obtained numerically on a quadrature grid that is used to compute the integrals in the GPU. The optimal computation is more than twenty times faster in the GPU than the calculation in CPU. The method can be easily scaled to computers with several Graphics Processing Units or clusters.
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1. Getting started

The properties of atoms and molecules can be determined by their wave function, which is obtained as the solution of the Schrödinger equation for non-relativistic energies. There are many methods to solve this second order, partial differential equation, from simple approximations that can give a hint of the physics, to the complete ab-initio numerical solution to predict physical quantities with a high degree of precision. When the wave function of an atomic or molecular system is written in a basis expansion, the Schrödinger equation transforms into a linear problem described by a dense matrix [1]. To obtain this matrix, it is necessary to compute integrals between two elements of the basis (called overlaps) and integrals of the interparticle potentials, that usually involve four basis functions.

The details of the calculation of each element of this matrix (called the Hamiltonian matrix) greatly depend on two factors. First, the system of coordinates chosen to represent the positions of the particles and their interactions, and second, the election of the basis set for each particle. These choices are determined not only by the number or type of particles involved, but also for the kind of experiment and/or physical property under investigation. For example, the simpler method makes use of Slater Type Orbitals (exponentials times powers of the electronic coordinates relative to the nuclei) as a basis set [2]. ... was used to study bound atomic systems, but not to analyze problems where particles can be spread out through the space, like ionization processes. Quantum chemistry calculations usually employ Gaussian functions to obtain properties of molecules, and take great advantage from the fact the systems under scrutiny are bound states [3–5].

Unlike these calculations of the quantum chemistry arena, collisional problems deal with particles that can be far from each other. In fact, the most important feature of a collision, the cross sections, are defined in those regions, assuming that the interactions among the particles are no longer effective and that they are far away from where the collision took place [6]. Therefore, the basis in collision problems should be able to accurately expand the full wave function for large interparticle distances. Moreover, if charged particles are present, the basis should take into account the long-range asymptotic behavior of Coulomb fields [7,8]. Finally, possibly the main shortcoming is that it is not possible to use simple analytic basis sets for collision problems. All these factors pose several challenges to perform a numerically accurate calculation of wave functions and cross sections in atomic and molecular collisions [9].

In the last few years, the computer hardware and software have been moving fast to an heterogeneous world [10]. In the desktop market, this meant going from a simple one-core desktop computer to an aggregate of one to several multicore CPUs with their corresponding accelerators. This also replicates in High Performance Computing clusters, such as the Titan supercomputer at Oak Ridge National Laboratory [11]. Nowadays it is not possible to program a scientific code thinking only about the pure speed of the calculation (i.e., floating points operations per second). In-core and out-of-core communication layers, memory hierarchies,

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J. Phys. B: At. Mol. Opt. Phys. 43 (2010) 101001 (5pp) doi:10.1088/0953-4075/43/10/101001

FAST TRACK COMMUNICATION

A boundary adapted spectral approach for breakup problems

A L Frapiccini[1], J M Randazzo[1], G Gasaneo[2] and F D Colavecchia[1]
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Abstract
We present a spectral method to study three-body fragmentation processes. The basis set explicitly includes continuum asymptotic boundary conditions and it is built upon generalized Sturmian functions. These functions are eigenvectors of a two-body problem where the magnitude of a potential is assumed as the eigenvalue. Comparison with a simple solvable analytical model demonstrates that our approach rapidly converges to the exact results, with basis sizes much smaller than other previous calculations. Preliminary calculations of H ionization by electron impact in the $L = 0$ approximation suggest that these convergence properties also apply to long-range Coulomb problems.

(Some figures in this article are in colour only in the electronic version)

PHYSICAL REVIEW A 82, 042503 (2010)

Sturmian expansions for two-electron atomic systems: Singly and doubly excited states

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PHYSICAL REVIEW A 87, 042707 (2013)

S-model calculations for high-energy-electron-impact double ionization of helium

In this paper the double ionization of helium by high-energy electron impact is studied. The corresponding four-body Schrödinger equation is transformed into a set of driven equations containing successive orders in the projectile-target interaction. The transition amplitude obtained from the asymptotic limit of the first-order solution is shown to be equivalent to the familiar first Born approximation. The first-order driven equation is solved within a generalized Sturmian approach for an S-wave (e,3e) model process with high incident energy and small momentum transfer corresponding to published measurements. Two independent numerical implementations, one using spherical and the other hyperspherical coordinates, yield mutual agreement. From our ab initio solution, the transition amplitude is extracted, and single differential cross sections are calculated and could be taken as benchmark values to test other numerical methods in a previously unexplored energy domain.

DOI: 10.1103/PhysRevA.87.042707 PACS number(s): 34.80.Dp, 34.50.−s

PHYSICAL REVIEW A 00, 002700 (2014)

Insights from the zero-angular-momentum wave in single and double ionization of He by fast electrons

Computer Physics Communications 182 (2011) 1145–1155
Contents lists available at ScienceDirect
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www.elsevier.com/locate/cpc

Computational methods for Generalized Sturmians basis

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Continuum spectra

ABSTRACT
The computational techniques needed to generate a two-body Generalized Sturmian basis are described. These basis are obtained as a solution of the Schrödinger equation, with two-point boundary conditions. This equation includes two central potentials: A general auxiliary potential and a short-range generating potential. The auxiliary potential is, in general, long-range and it determines the asymptotic behavior of all the basis elements. The short-range generating potential rules the dynamics of the inner region. The energy is considered a fixed parameter, while the eigenvalues are the generalized charges. Although the finite differences scheme leads to a generalized eigenvalue matrix system, it cannot be solved by standard computational linear algebra packages. Therefore, we developed computational routines to calculate the basis with high accuracy and low computational time. The precise charge eigenvalues with more than 12 significant figures along with the corresponding wave functions can be computed on a single processor within seconds.
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PHYSICAL REVIEW A 84, 052715 (2011)

Solving three-body-breakup problems with outgoing-flux asymptotic conditions

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(Received 21 June 2011; published 17 November 2011)

An analytically solvable three-body collision system (s wave) model is used to test two different theoretical methods. The first one is a configuration interaction expansion of the scattering wave function using a basis set of Generalized Sturmian Functions (GSF) with purely outgoing flux (CISF), introduced recently in A. L. Frapiccini, J. M. Randazzo, G. Gasaneo, and F. D. Colavecchia [J. Phys. B: At. Mol. Opt. Phys. 43, 101001 (2010)]. The second one is a finite element method (FEM) calculation performed with a commercial code. Both methods are employed to analyze different ways of modeling the asymptotic behavior of the wave function in finite computational domains. The asymptotes can be simulated very accurately by choosing hyperspherical or rectangular contours with the FEM software. In contrast, the CISF method can be defined both in an infinite domain or within a confined region in space. We found that the hyperspherical (rectangular) FEM calculation and the infinite domain (confined) CISF evaluation are equivalent. Finally, we apply these models to the Temkin-Poet approach of hydrogen ionization.

DOI: 10.1103/PhysRevA.84.052715 PACS number(s): 34.80.Dp, 31.15.−p, 34.10.+x

Few-Body Syst DOI 10.1007/s00601-014-0831-5

M. J. Ambrosio · L. U. Ancarani · D. M. Mitnik · F. D. Colavecchia · G. Gasaneo

A Generalized Sturmian Treatment of $(e, 3e)$ Processes Described as a Three-Body Coulomb Problem

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Abstract The double ionization of helium by high energy electron impact is investigated. The pure four-body Coulomb problem may be reduced to a three-body one in accordance with the use of the first Born approximation. Even within this frame, major unexplained discrepancies subsist between several theoretical descriptions and the available absolute experimental data. In this contribution we discuss an alternative formulation which allows to tackle the problem with a different methodology, the generalized Sturmian approach. We discuss some issues associated to the convergence of the calculated cross sections.

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Sturmian functions in a L^2 basis: Critical nuclear charge for N-electron atoms

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Available online 21 February 2007

Abstract
Two particle Sturmian functions [M. Rotenberg, Ann. Phys., NY 19 (1962) 262; S.V. Khristenko, Theor. Math. Fiz. 22 (1975) 31 (Engl. Transl. Theor. Math. Phys. 22, 21)] for a short range potentials are obtained by expanding the solution of the Schrödinger equation in a finite L^2 Laguerre-*type* basis. These functions are chosen to satisfy certain boundary conditions, such as regularity at the origin and the correct asymptotic behavior according to the energy domain: exponential decay for negative energy and outgoing (incoming or standing wave) for positive energy. The set of eigenvalues obtained is discrete for both positive and negative energies. This Sturmian basis is used to solve the Schrödinger equation for a one-particle model potential [A.V. Sergeev, S. Kais, J. Quant. Chem. 75 (1999) 533] to describe the motion of a loosely bound electron in a multielectron atom. Values of the two parameters of the potential are computed to represent the Helium isoelectronic series and the critical nuclear charge Z_c is found, in good agreement with previous calculations.
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Keywords: Sturmian functions; Critical nuclear charge; N-electron atoms

1. Introduction

The Sturmian functions [1,2] for a two-body system are of particular interest in atomic physics. These functions are solutions of the two-body Schrödinger equation for some physical potential, where the energy is fixed and the strength of the potential is the eigenvalue. Besides, they satisfy a set of boundary conditions of the physical problem to be solved. Negative energy Sturmians that decay exponentially at large distances make a discrete basis for negative energies, and have been widely used in atomic physics to determine atomic energy levels [4–6], or to expand the Coulomb Green function (see [7] and references therein).

Meanwhile, at positive energies, Sturmian functions might be defined to satisfy outgoing, incoming or standing wave boundary conditions. The spectrum of eigenvalues thus depend on the choice of the asymptotic behavior of the eigenfunction. Ovchinnikov and Macek [8] obtained a discrete set of eigenvalues for purely outgoing wave Sturmians, however this functions became unbounded as r increased. Rawitscher [9] was able to define a set of Sturmians with outgoing wave condition even in the case where a long range potential was present, showing that they constitute a discrete basis set with discrete eigenvalues.

Following this approach, we propose a systematic method to obtain Sturmian functions for both negative and positive energies, expanding the solution of the radial part of the Schrödinger equation in a L^2 Laguerre-*type* basis set. The use of the Green's function ensures the asymptotic behavior in the entire energy domain. This basis set is therefore suitable for constructing the wave function of a given scattering problem for both long range Coulomb potentials or short range potentials.

In Section 1 of this paper we present a brief review of the Sturmian theory and an analysis of the different asymptotic behavior according to the energy domain. In Section 2 we outline the general method to expand the two-particle Sturmian functions in terms of Laguerre-*type* basis, and obtain orthogonality and closure relations restricted to a finite subspace. Numerical results for a Coulomb well potential are shown for both negative and positive energies. In Section 3 we use the

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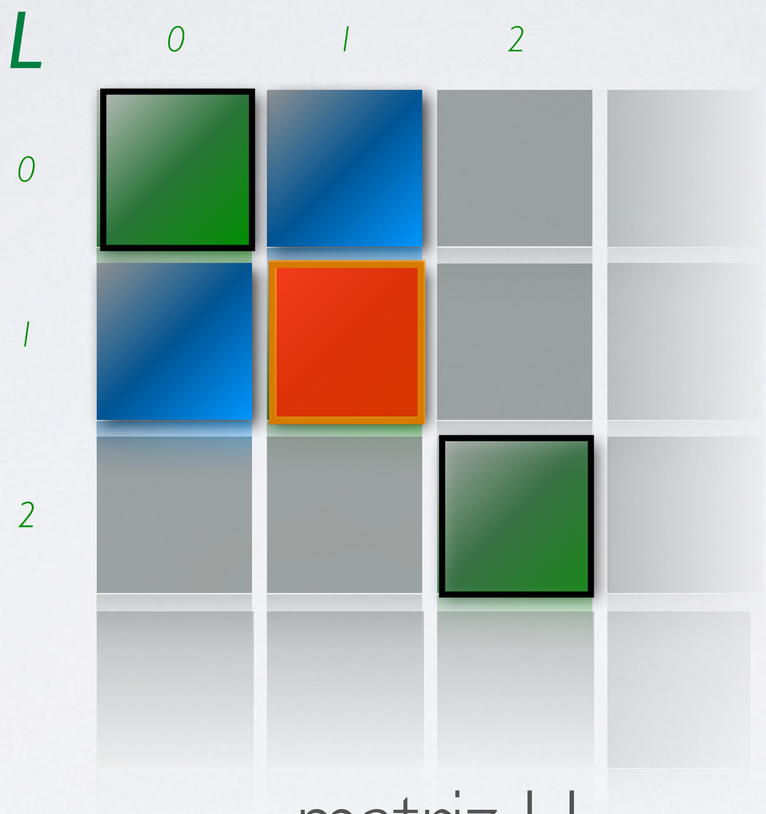
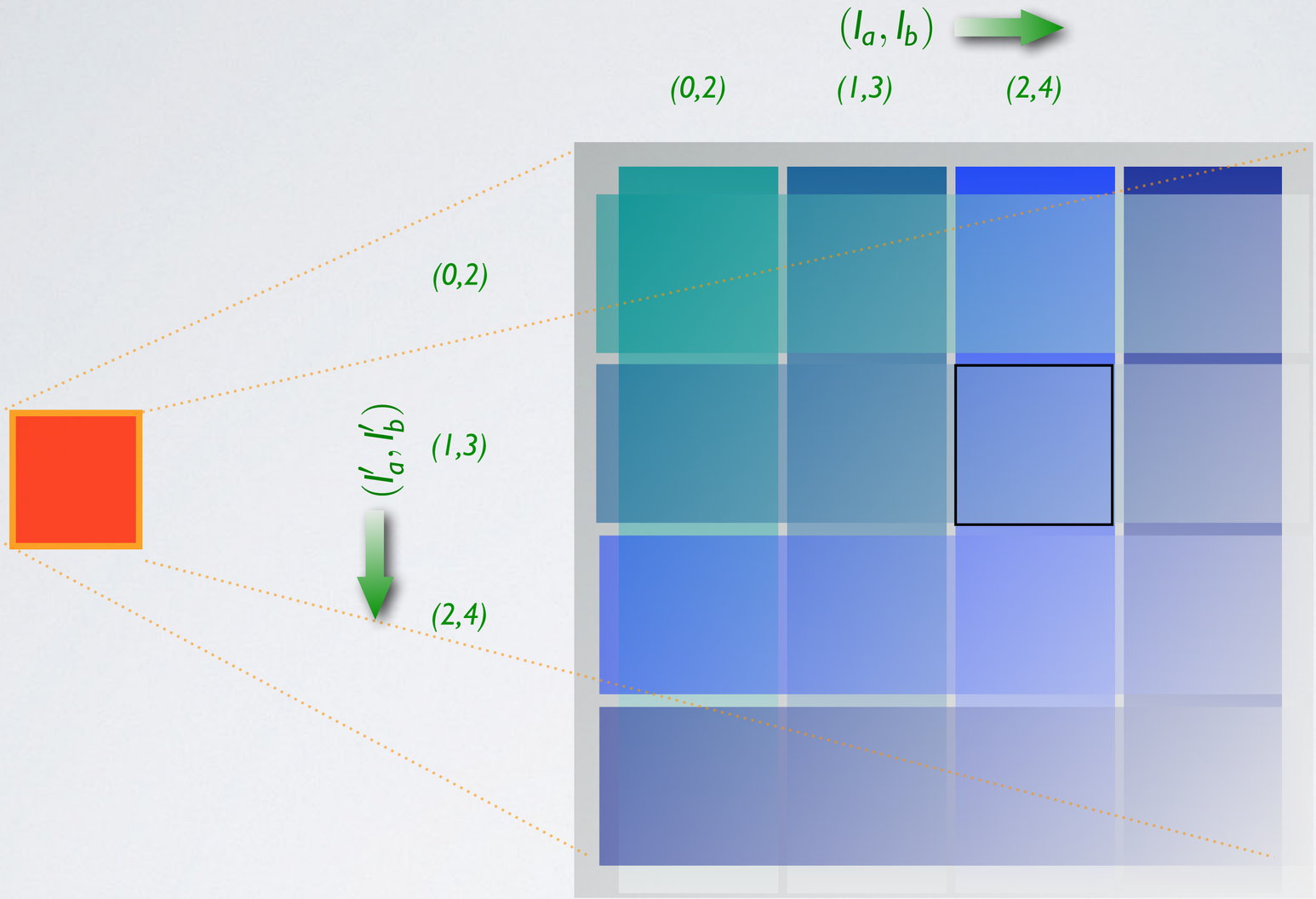
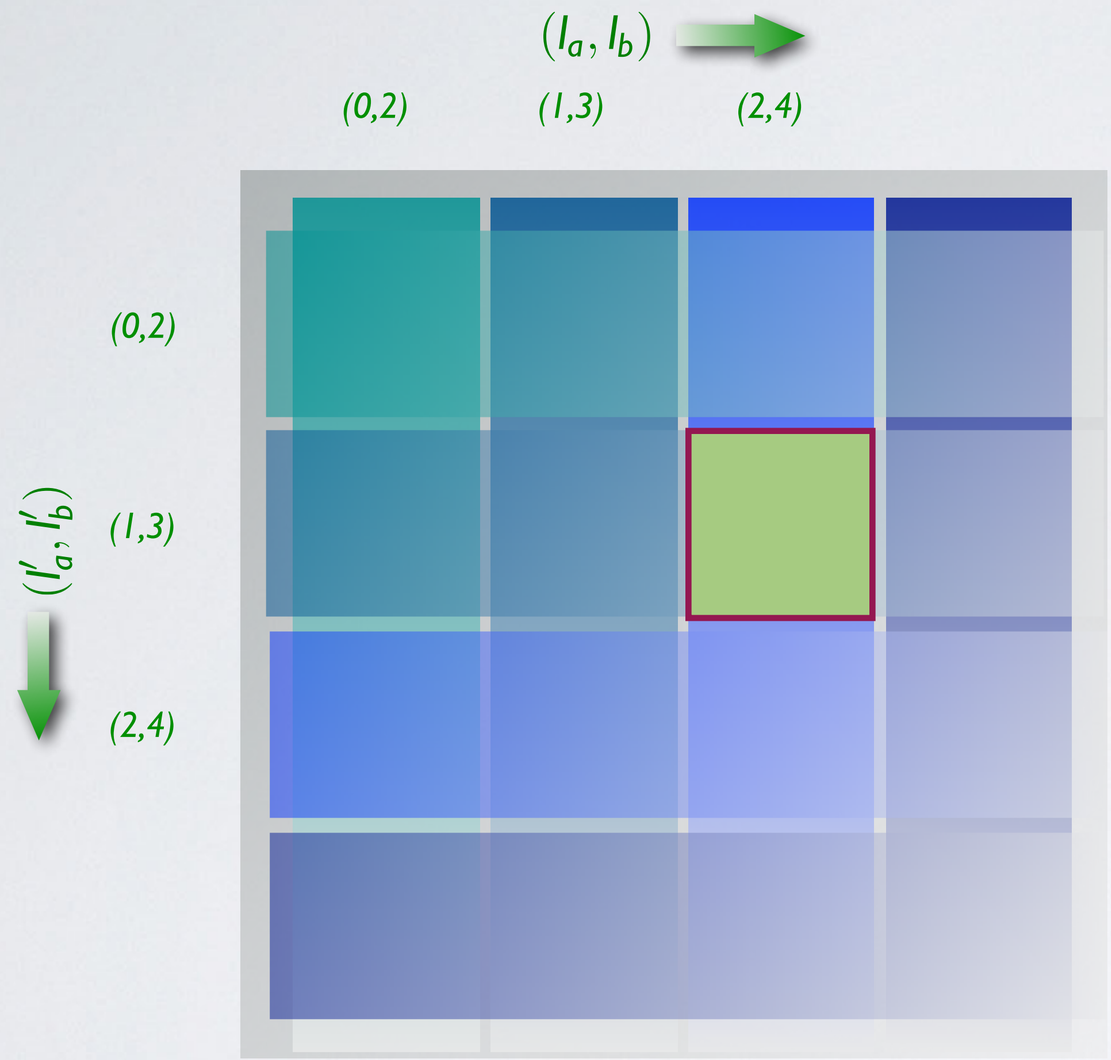


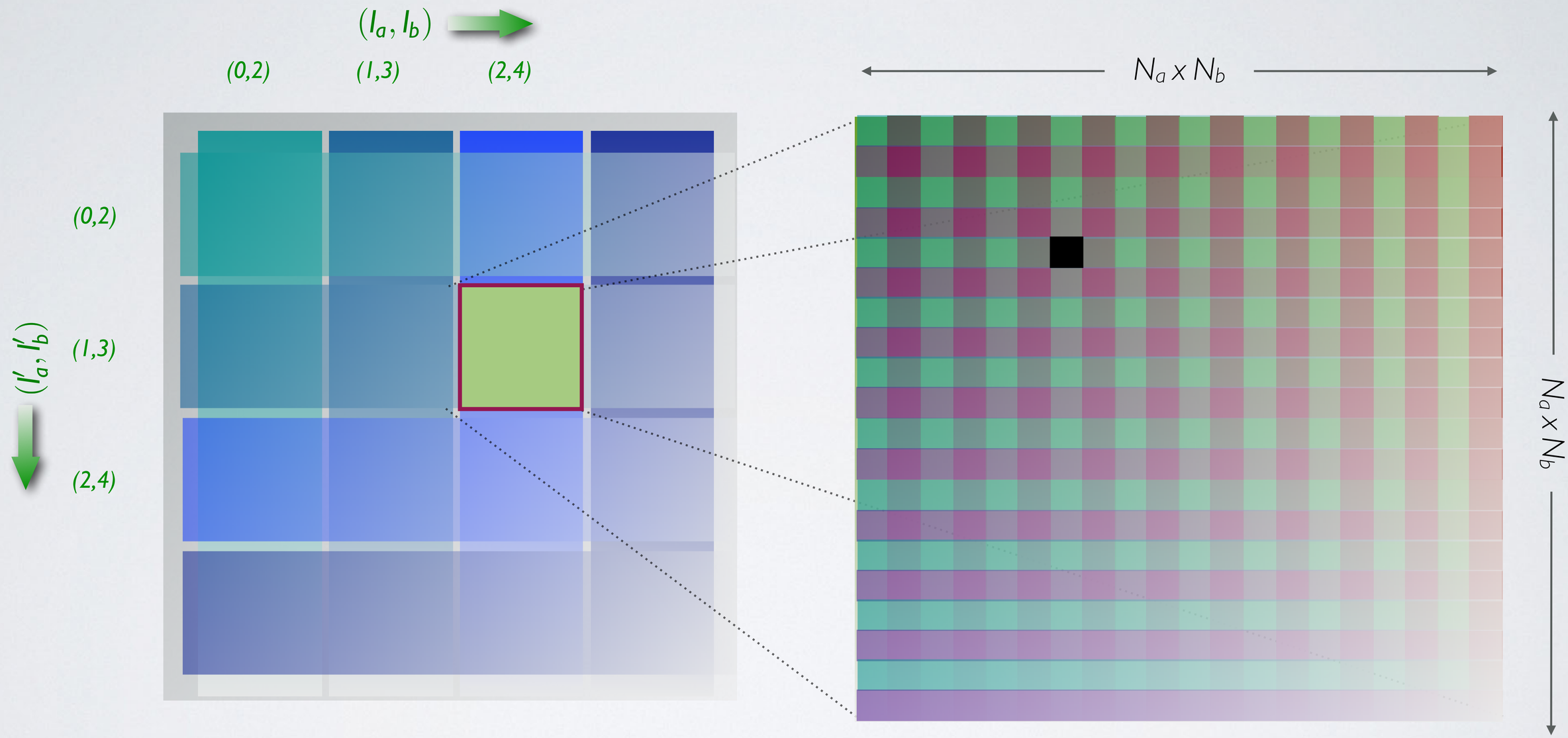
matriz H
bloques de L

bloque de L fijo



bloque de L fijo


(l_a, l_b)
(0,2)
(1,3)
(2,4)
(0,2)
(1,3)
(2,4)
(l'_a, l'_b)


(l_a, l_b)
(0,2)
(1,3)
(2,4)
$N_a \times N_b$
(0,2)
(1,3)
(2,4)
(l'_a, l'_b)
$N_a \times N_b$

Cada elemento de matriz H tiene

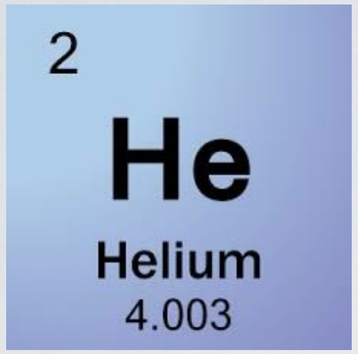
2 integrales 1D (overlaps) prod. escalar

n integrales 2D (repulsión) prefix sum
prod. escalar

0

1

2

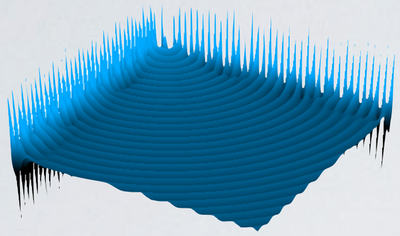


$L=0$ x 13 pares (l_a,l_b) x $n=2$ x $N_a=N_b=35$

1 x 13 x 13 x 2 x 1225 x 1225

253 605 625 2D

4 GB



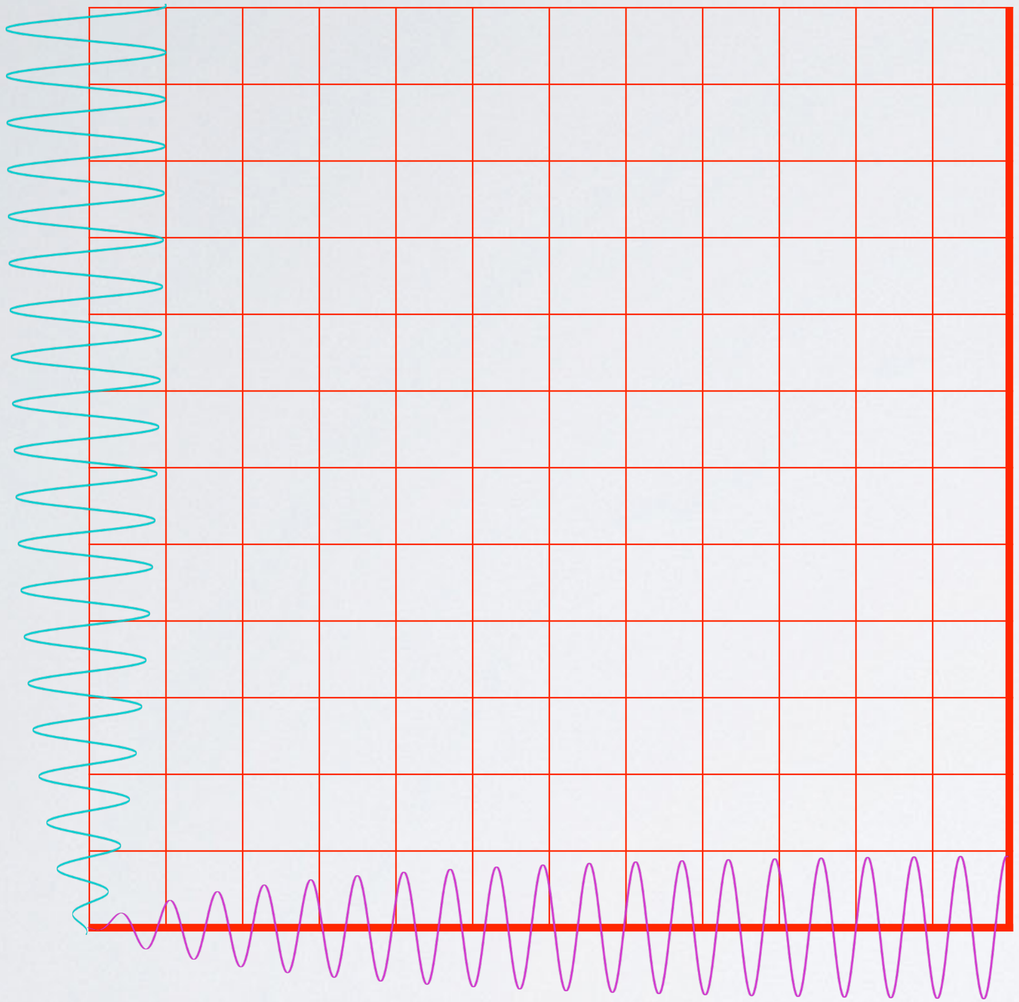
colisión (e,3e)

$L=0\text{-}4 \quad \times \quad 5 \text{ pares } (l_a,l_b) \quad \times \quad n=2 \quad \times \quad N_a=N_b=84$

$5 \quad \times \quad 5 \times 5 \quad \times \quad 2 \quad \times \quad 7056 \times 7056$

12 446 784 000 2D

98 GB



dominio radial finito (2D) + C. C.

método espectral

cálculo de la matriz H

problema de álgebra lineal numérica denso

cálculo de la
matriz H

C + Fortran + CUDA

14 000 000 2D/s

25 x

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Accelerating spectral atomic and molecular collisions methods with graphics processing units

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ABSTRACT

We present a computation method to accelerate the calculation of the Hamiltonian of a three-body time independent Schrödinger equation for collisions. The Hamiltonian is constructed with one dimensional (basis overlaps) and two dimensional (interparticle interaction) integrals that are mapped into a computational grid in a Graphics Processing Unit (GPU). We illustrate the method for the case of an electron impact single ionization of a two electron atom. This proposal makes use of a Generalized Sturmian Basis set for each electron, which are obtained numerically on a quadrature grid that is used to compute the integrals in the GPU. The optimal computation is more than twenty times faster in the GPU than the calculation in CPU. The method can be easily scaled to computers with several Graphics Processing Units or clusters.

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problema de álgebra lineal numérica denso

Fortran + MPI + ScaLapack

d. mitnik

north carolina (EE UU)
metz (Francia)

cálculo de la
matriz H

+

problema de álgebra
lineal numérica
denso

C + Fortran + CUDA

MPI

Fortran + MPI + ScaLapack

producción
1er semestre 2015

$$e + H \longrightarrow e + H^{+} + e$$

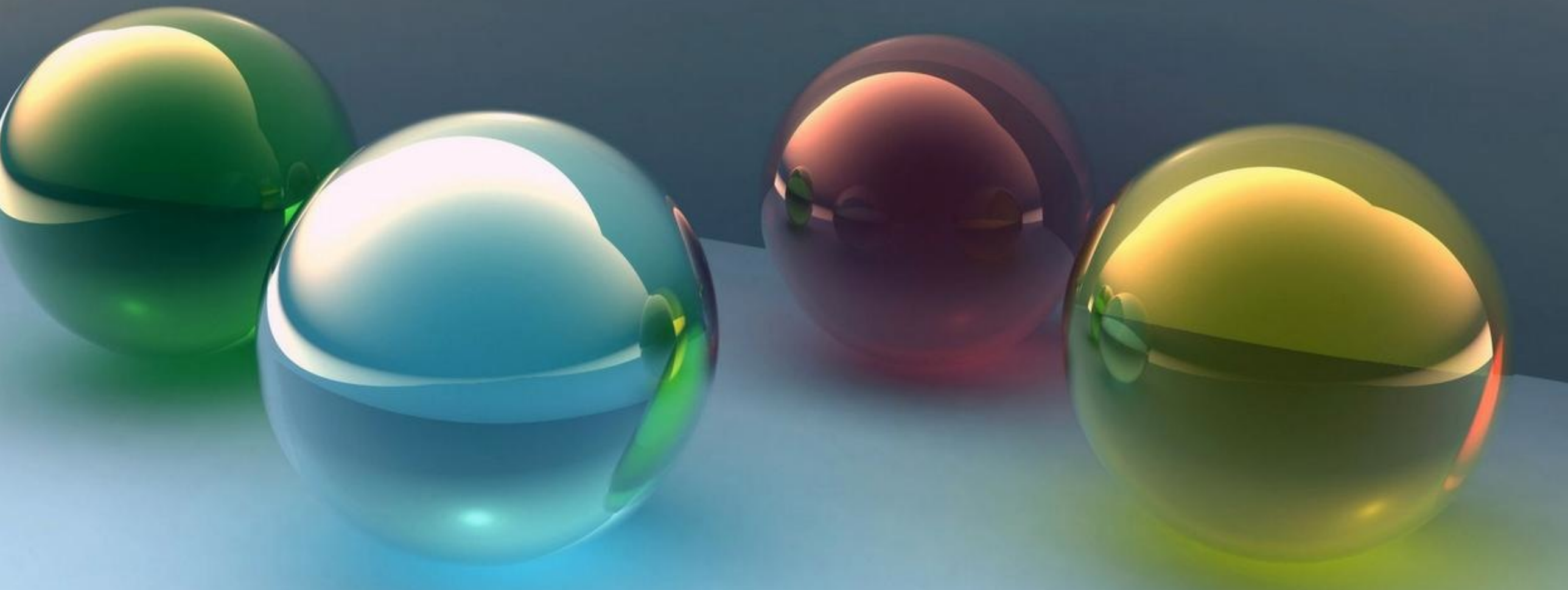
$$e + W^{q+} \longrightarrow e + W^{q+l} + e$$

$$h\nu + He@C_{60} \longrightarrow e + He@C_{60}{}^{++} + e$$

$$H_2 + H \longrightarrow H + H + H$$

4 cuerpos

30 TB



5 cuerpos …..

cálculo de la
matriz H

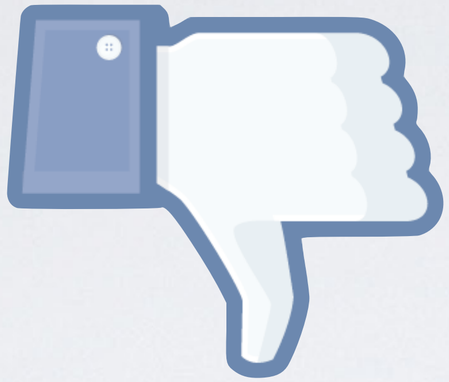
+

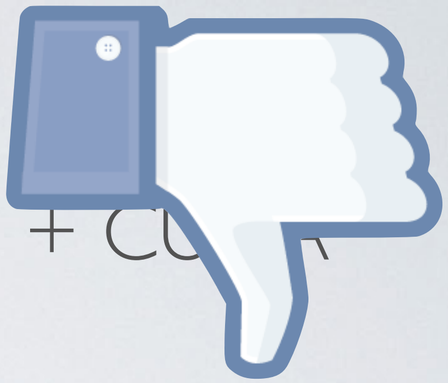
problema de álgebra
lineal numérica
denso

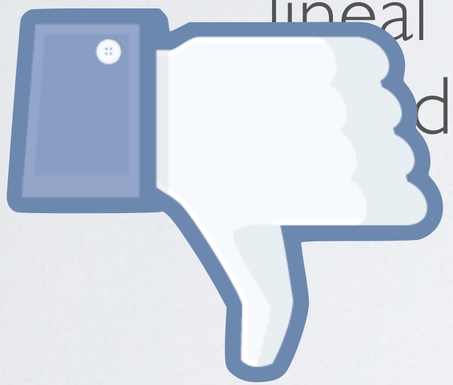
C + Fortran + CU[illegible]

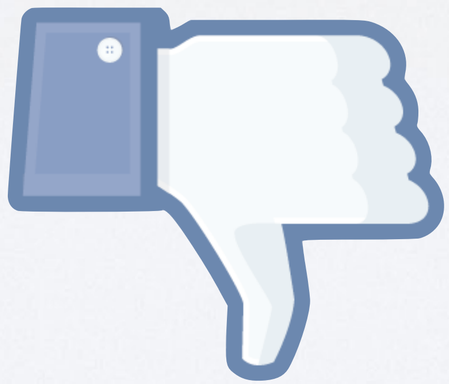
MPI

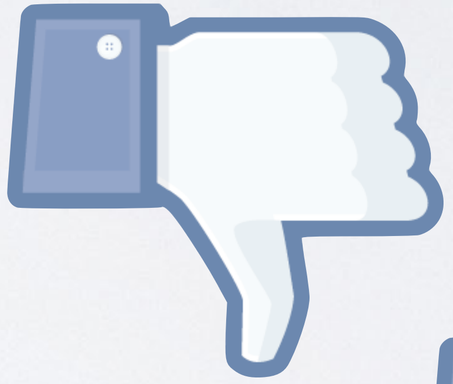
Fortran + MPI + ScaLapack

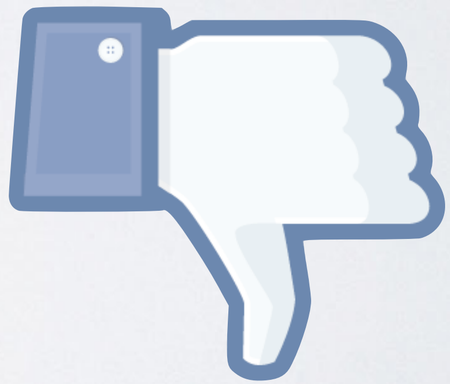












problema de álgebra
lineal numérica
denso

para

una matriz que no se conoce *a priori*

pero cuyos elementos se saben
calcular

matrices latentes

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