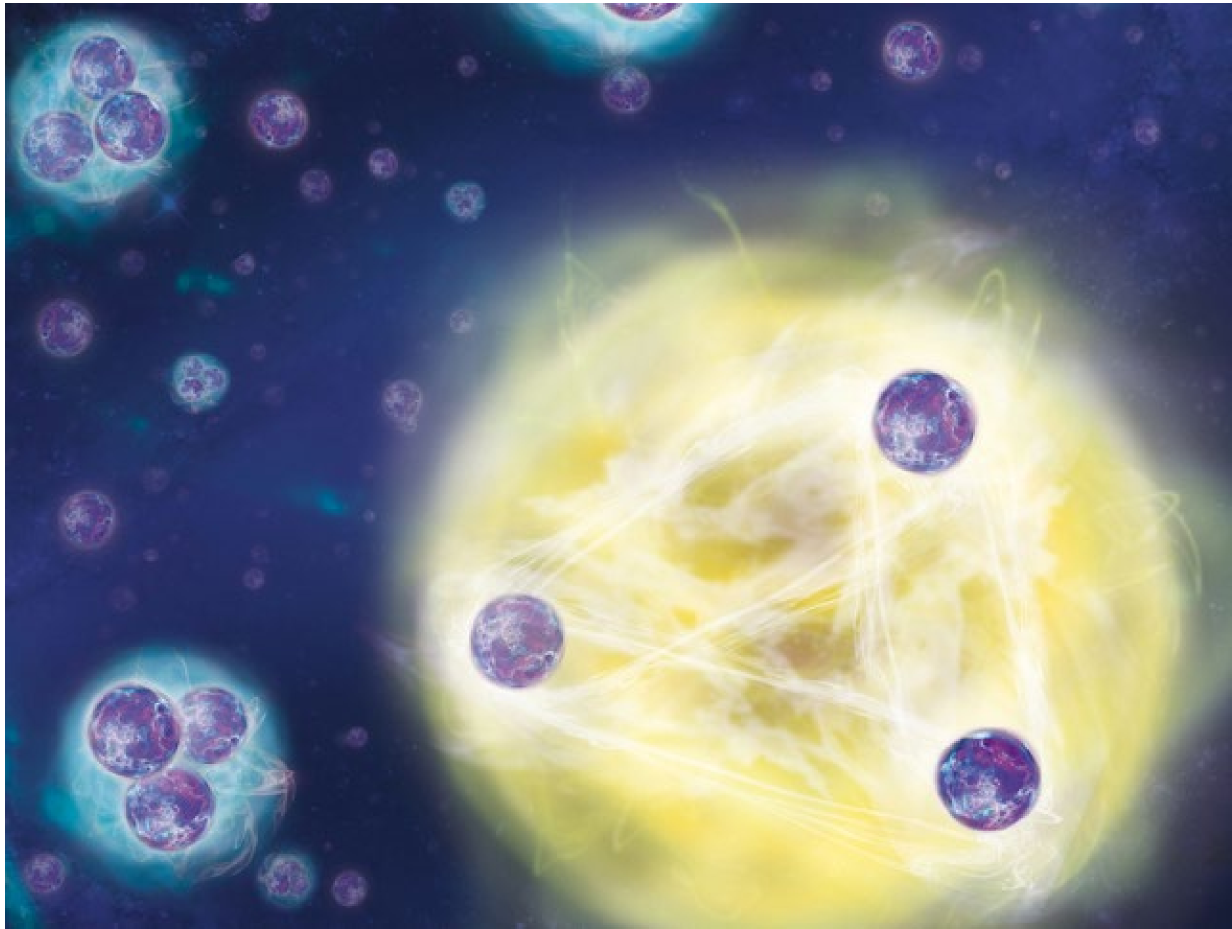
High performance simulation of strongly interacting three-body quantum systems

Jasper van de Kraats

Xavier Álvarez Farré

ACUD – 12/12/2024

Natalie Wolchover. Physicists prove surprising rule of threes. Quanta magazine (2014)



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Quantum *simulation*

Physics is hard,
can we make it
easier?

Quantum *simulation*

Quantum *simulation*

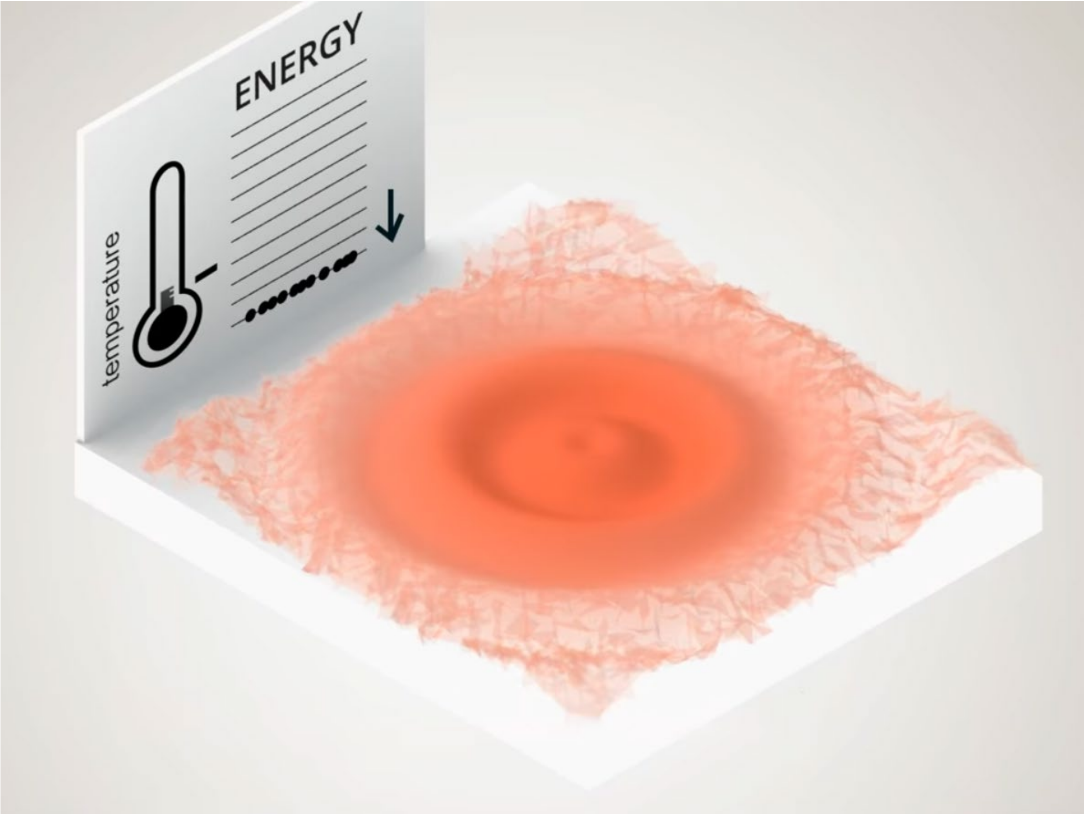
Shortly thereafter the physicist returned to the farm, saying to the farmer, "I have the solution, but it works only in the case of spherical cows in a vacuum."

https://en.wikipedia.org/wiki/Spherical_cow

Ultracold atomic gases

Ultracold atomic gases

$$T \sim 1 - 100 \text{ nK}$$



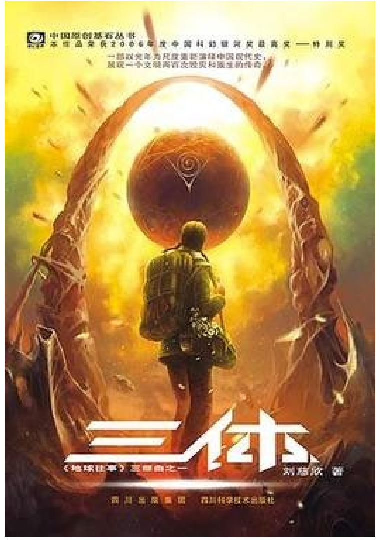
Julien Bobroff, Frédéric Bouquet and David Clément. www.quantummadesimple.com

Ultracold atomic gases provide:

- Universality
- Detectability
- Controllability

Ideal for quantum simulation!

The three-body problem



© Congqing press

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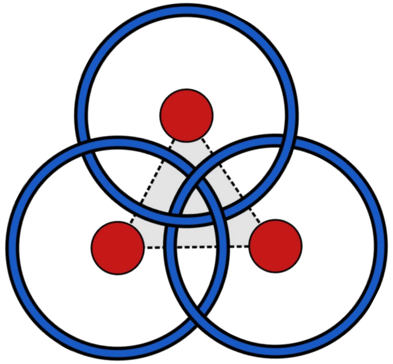
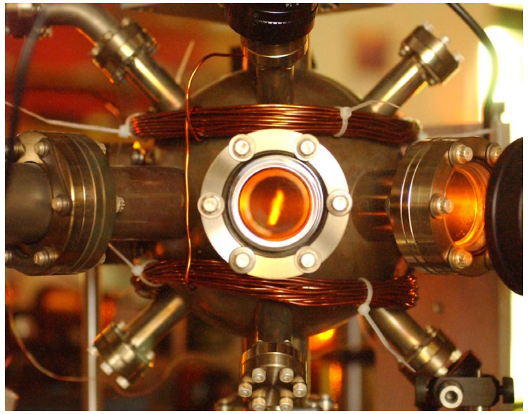
Instead of planets, let's think about atoms

The Efimov effect



Borromean bond

Vitaly Efimov (CERN, 2019)



Pomona College, Claremont, California. (2020, February 18). *Bose-Einstein Condensates*. Retrieved March 16, 2023

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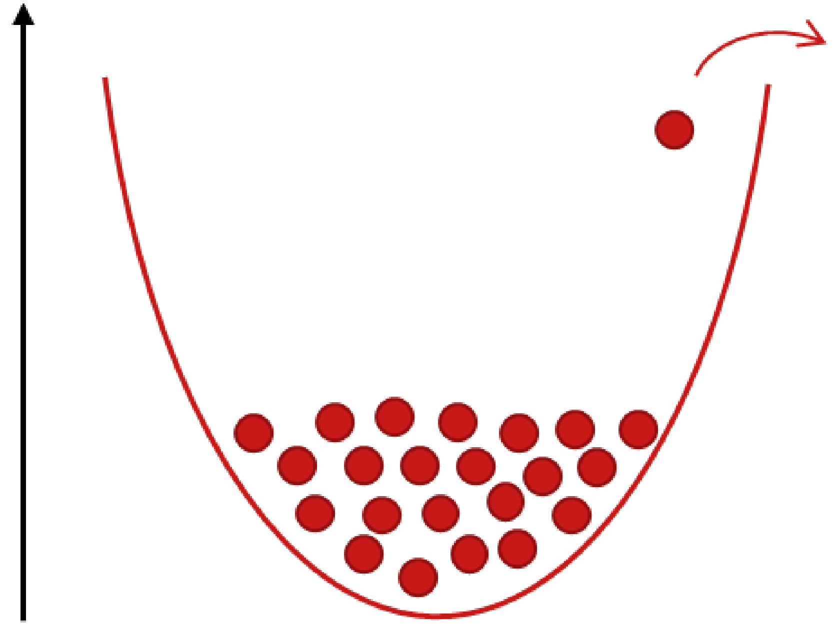
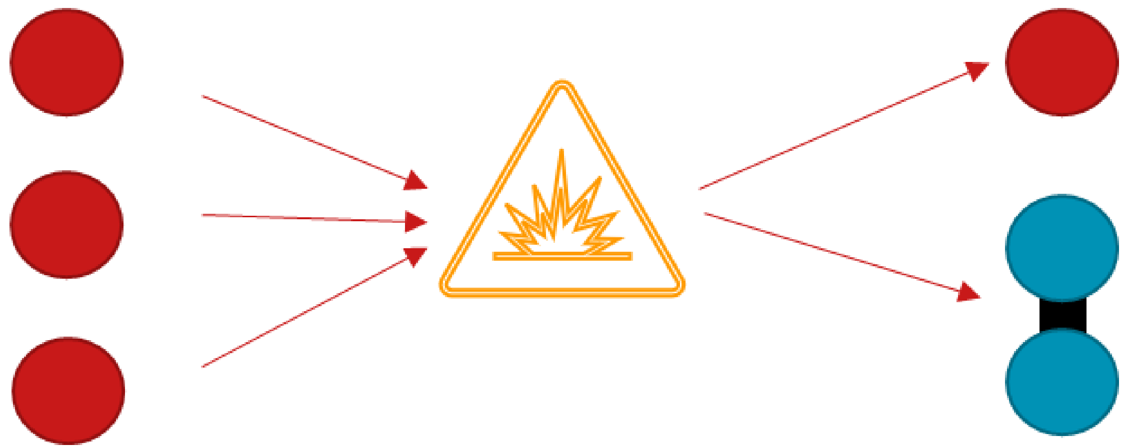
By NASA/CXC/SAO (X-Ray); NASA/JPL-Caltech (Infrared)

The probe: particle loss

Particle trap



Three-body recombination



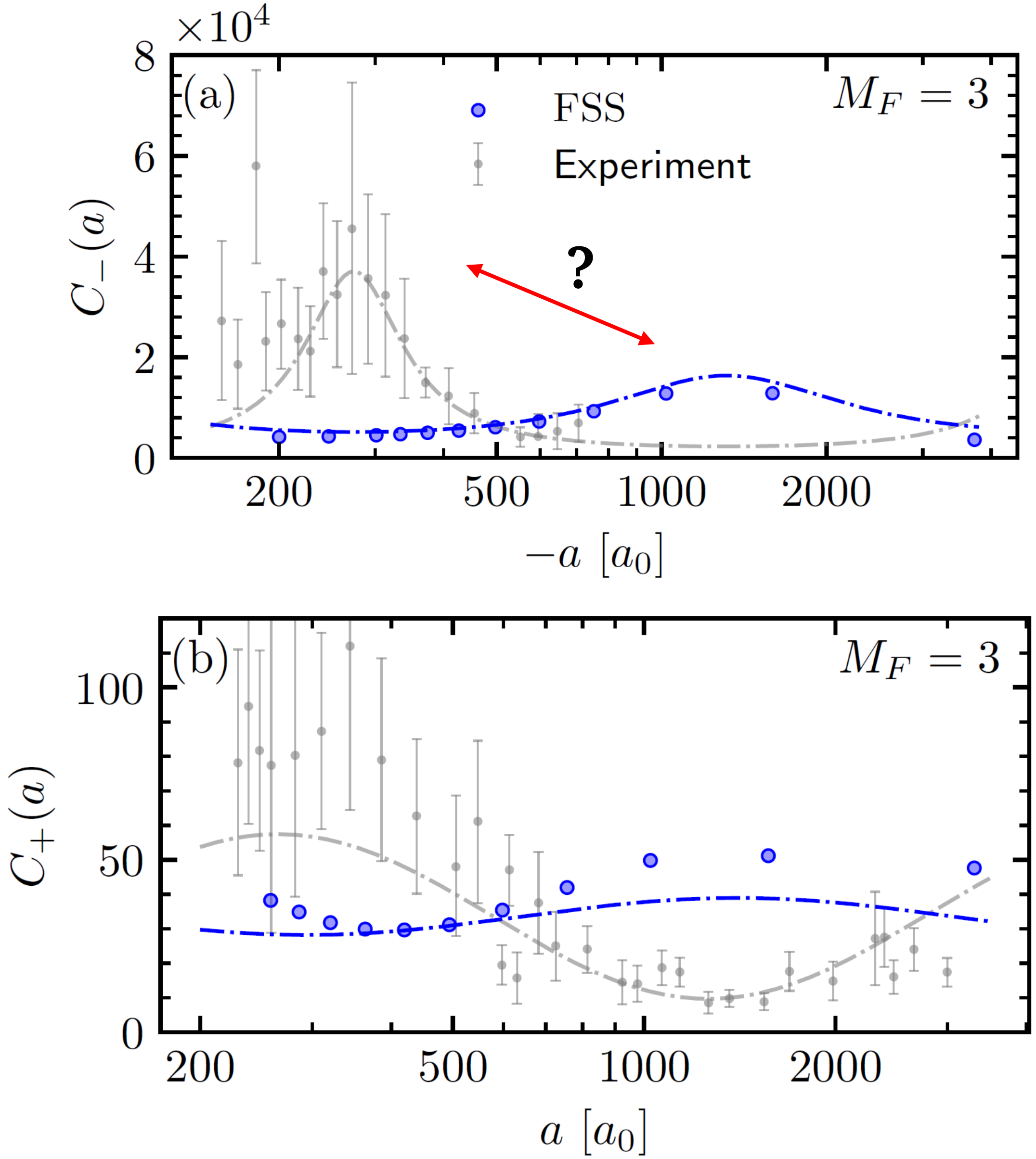
Sensitive to the Efimov effect!

Our goal: Solve the three-body problem to calculate three-body recombination rates

Problem statement

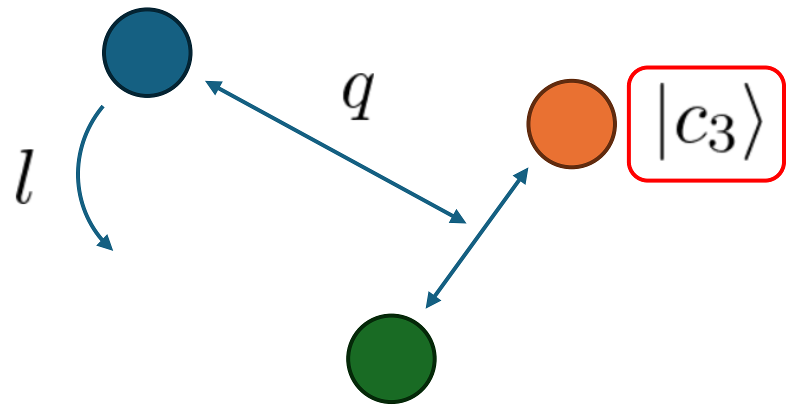
Lithium few-body puzzle

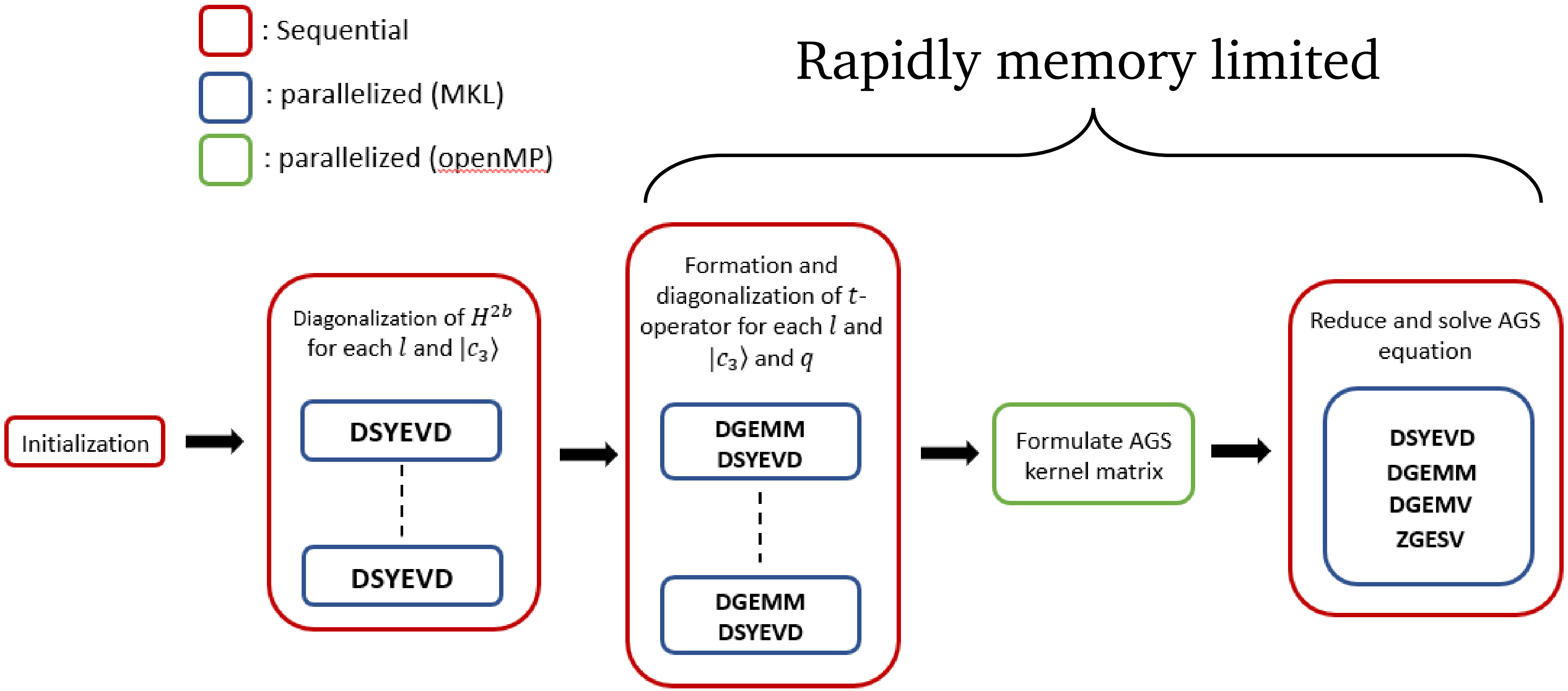
Unsolved problem in atomic physics for the last 14 years



Why HPC?

Degrees of freedom:





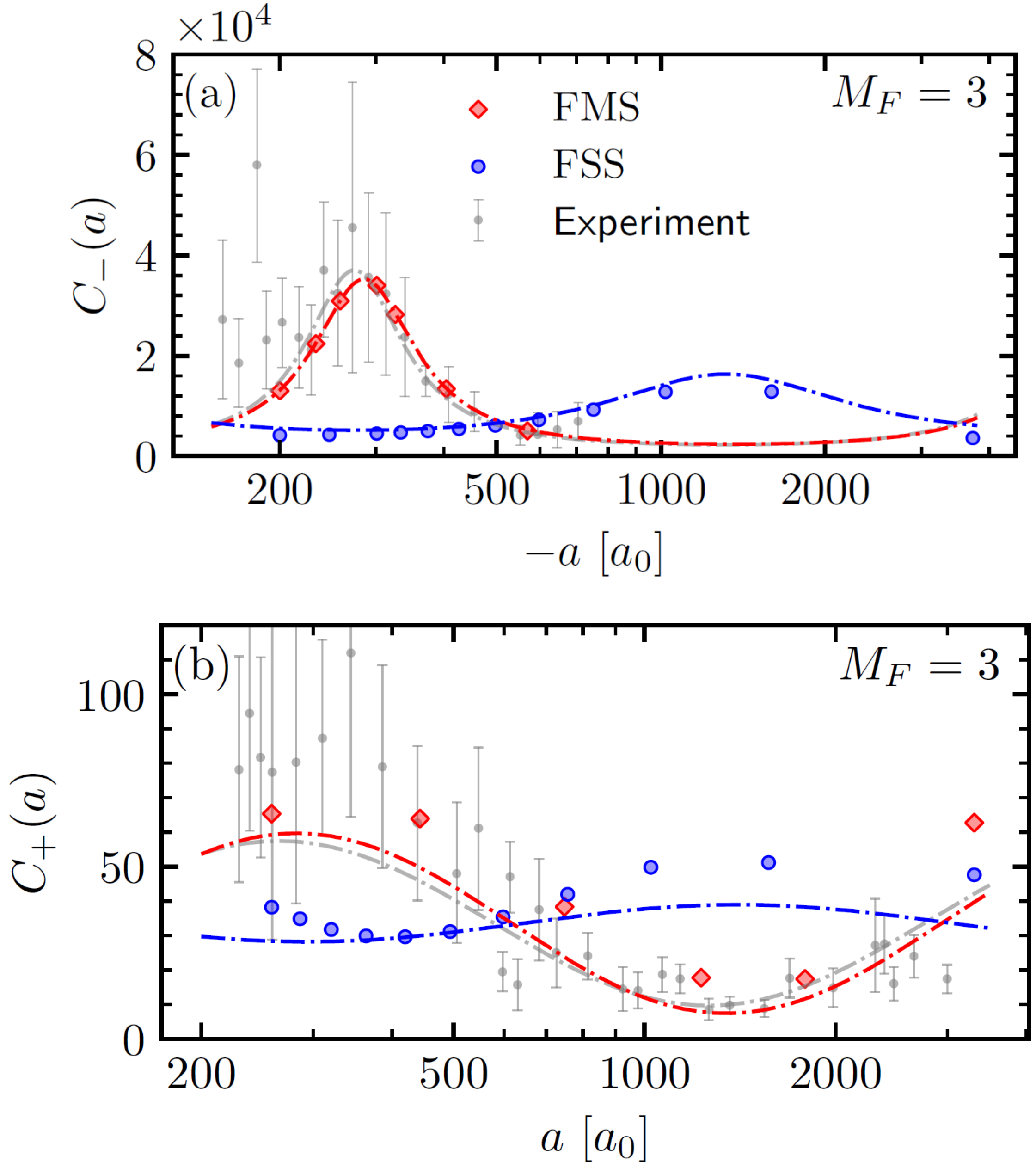
But does it work?

With aid of high-memory nodes on Snellius we were able to converge our numerical method for the first time, including all degrees of freedom

Obtained unprecedented match with experimental data

J. van de Kraats et. al., Phys. Rev. Lett. ***132****, 133402 (2024)*

J. van de Kraats et. al., Few-Body Syst. ***65****, 85 (2024)*



Parallel implementation of the simulation of strongly interacting three-body quantum systems

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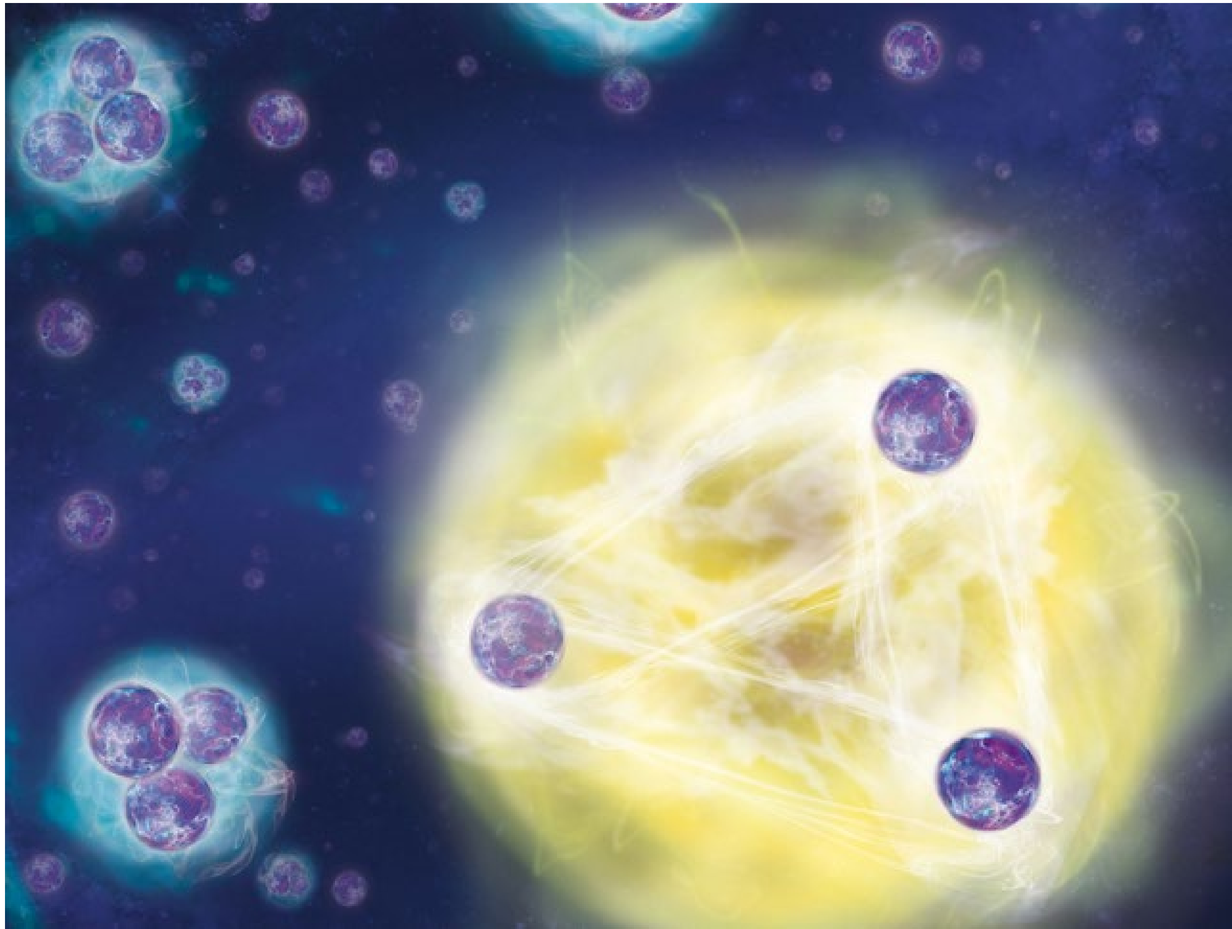


Baseline implementation

From a computational perspective, the three-body problem solver comprises **two primary routines**.

2-body

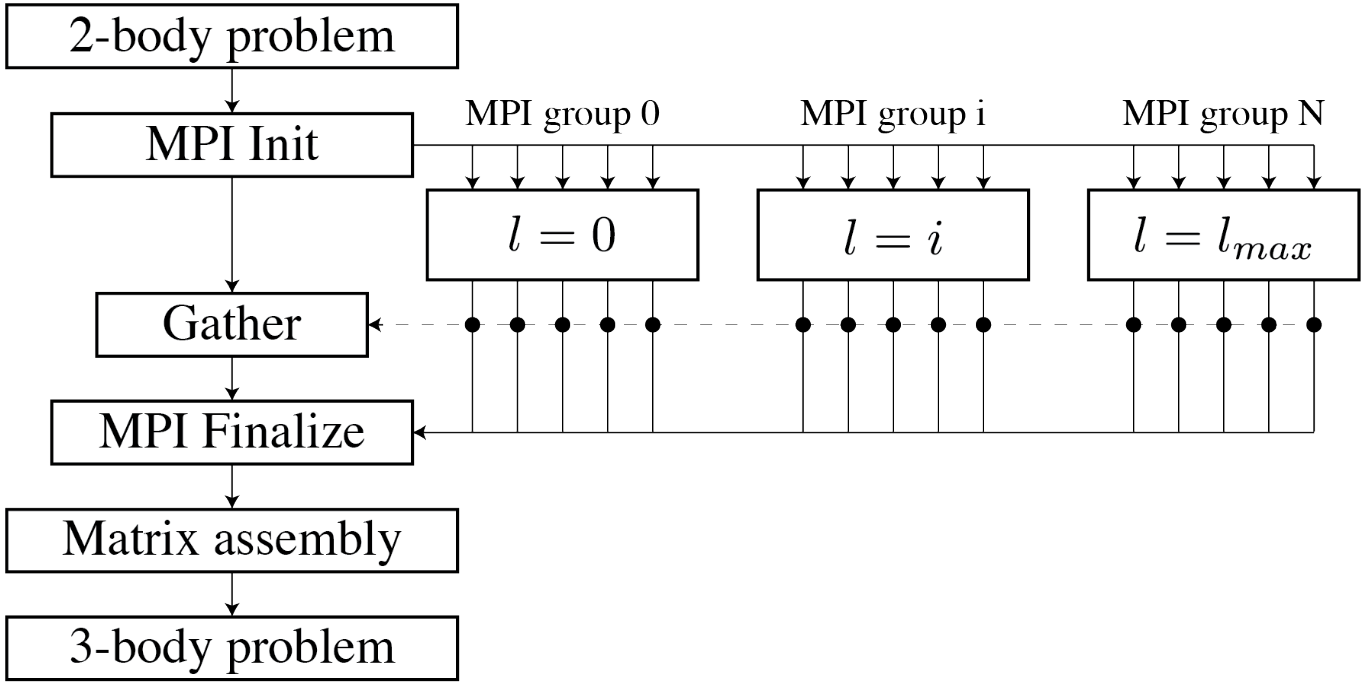
- Large set of independent 2-body calculations, which form the basis for assembling the matrix for solving the 3-body problem.

3-body

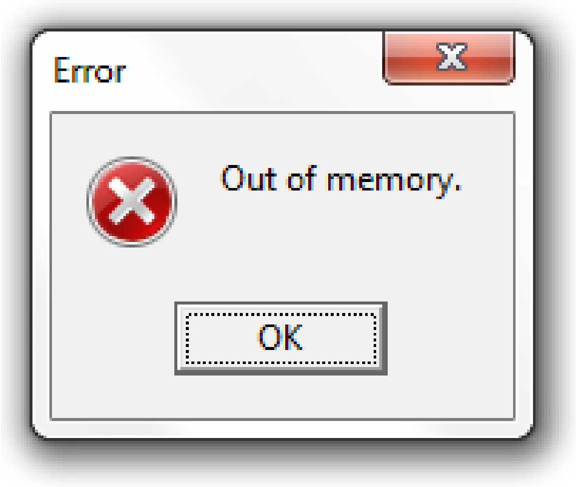
- Resolution of one large, dense linear algebra system.

Baseline implementation

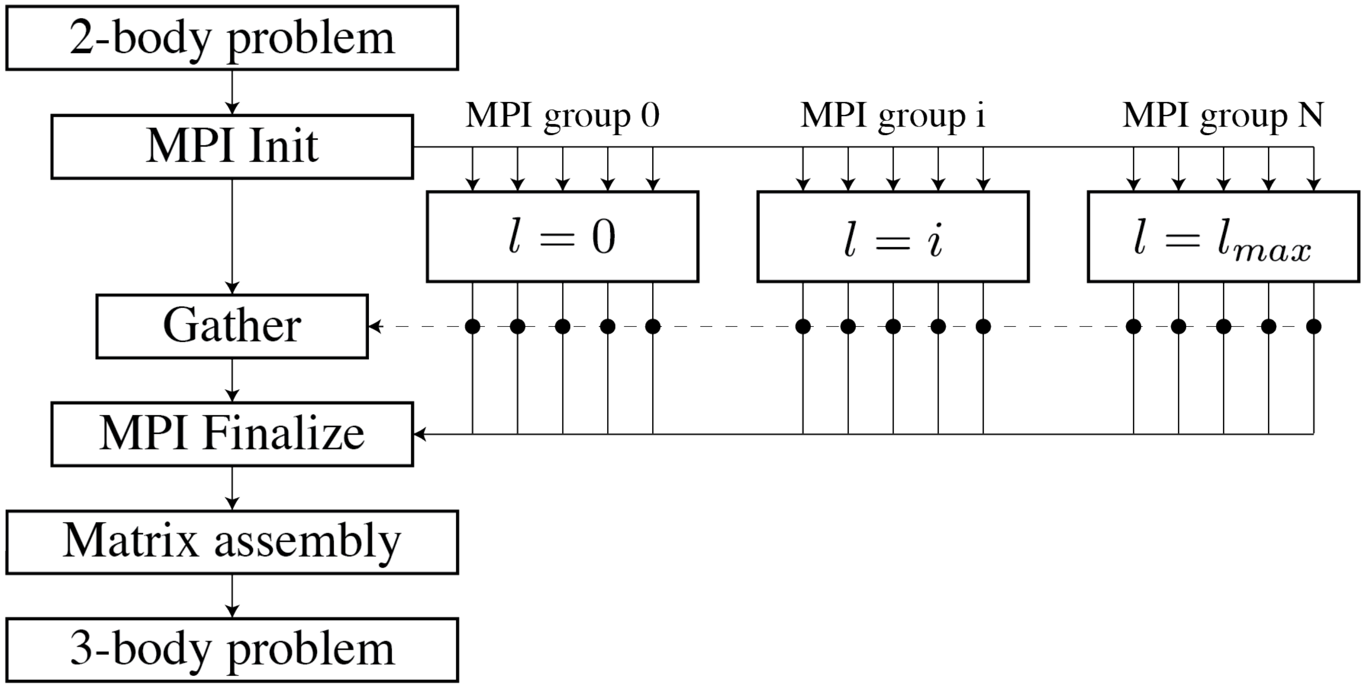
- The code is written in **Fortran 90**, with minimal dependencies.
- Calculations relying primarily on linear algebra routines from the **Intel Math Kernel Library** (MKL).
- Native multithreading (OpenMP) is provided by the library.
- Baseline MPI parallelization of the 2-body routine was heavily imbalanced.



Bottlenecks identified



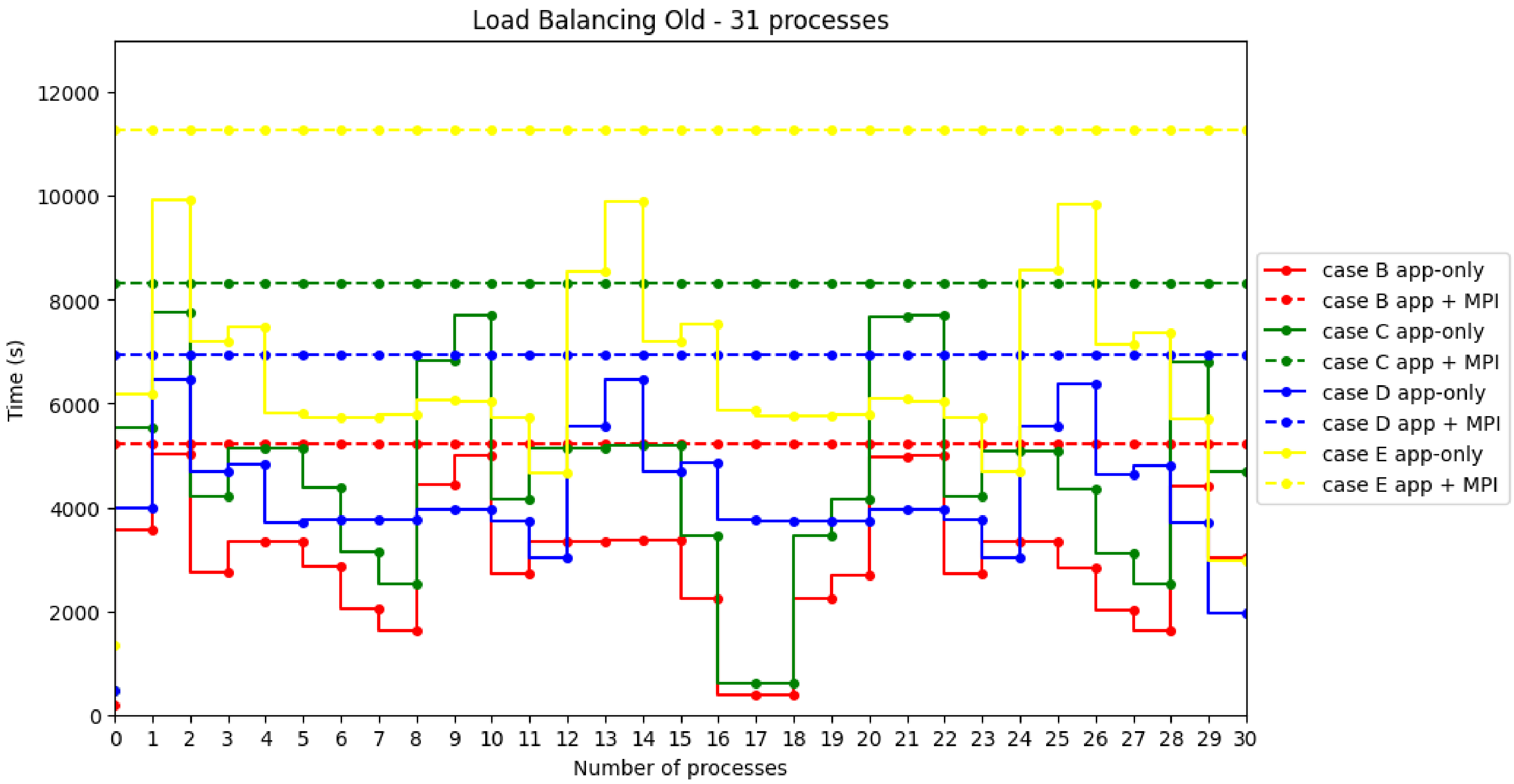
- **Memory**: 3-body routine limited to a single (high-memory) node, i.e., **8 TB** on Snellius.
- **Wall-clock time**: compute time limited to a single node, i.e., **128 cores** on Snellius.
- **Efficiency**: high **imbalance** in the 2-body routine.



MPI profiling of the 2-body routine

Baseline workload distribution follows a **physical rationale**:

- MPI processes are grouped into equally sized **groups assigned to different *l* values**.
- For each *l*, particle **states are evenly distributed among the processes** in the group

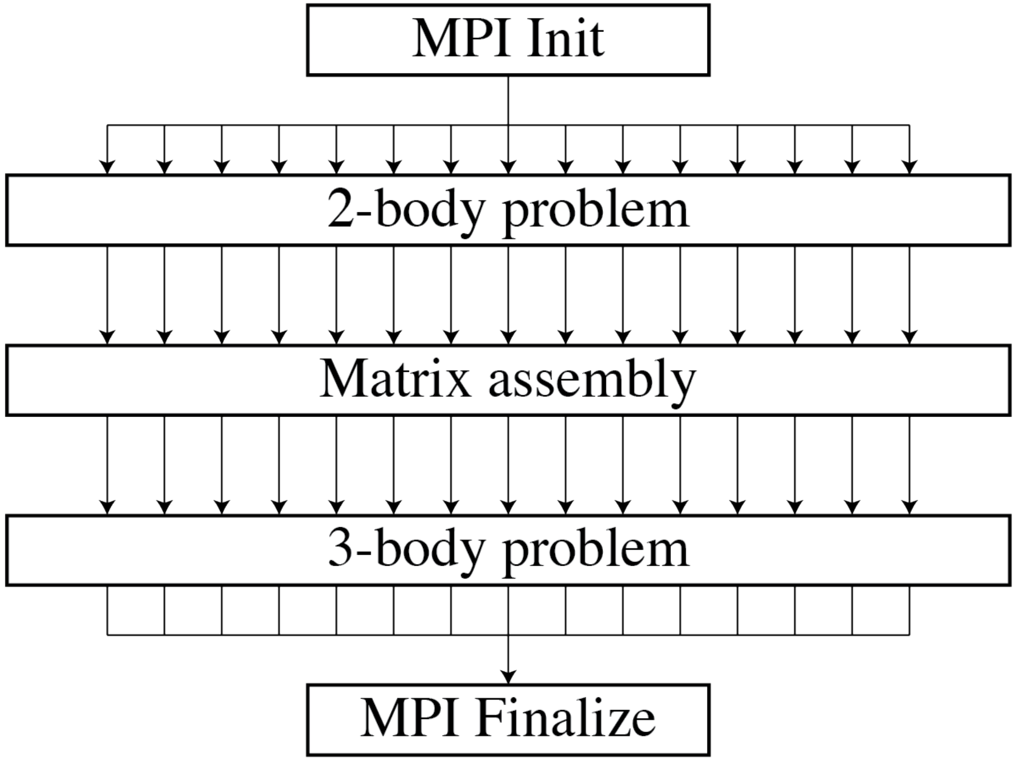


Baseline implementation

The goal is to upgrade the baseline to a **fully distributed parallel implementation**.

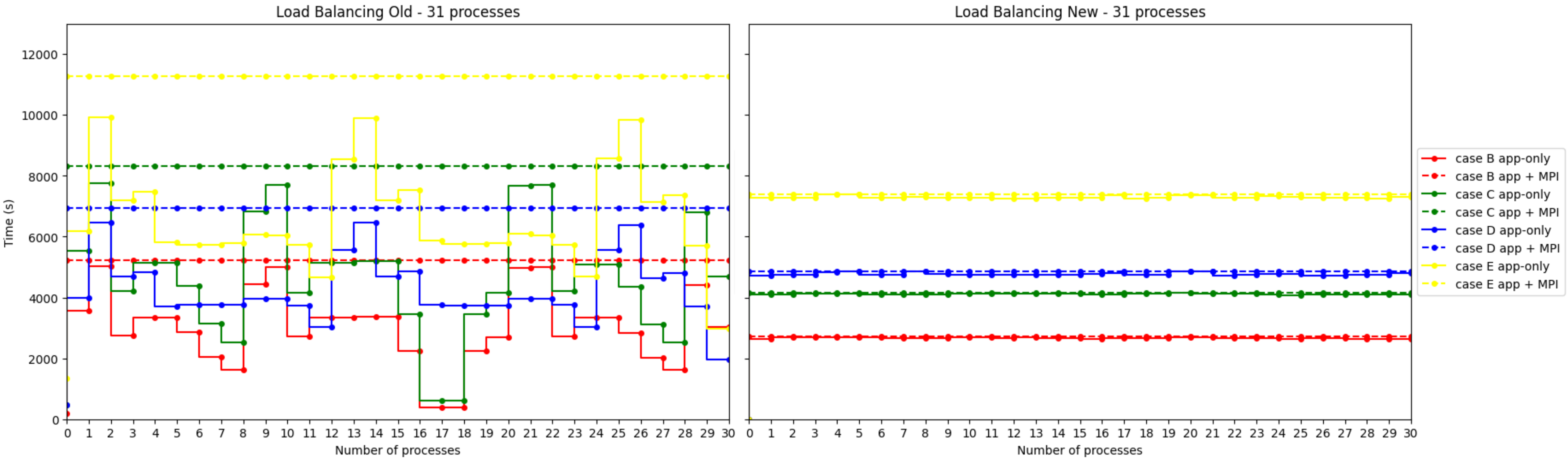
- **2-body routine**: tasks are distributed per worker process, reducing workload imbalance and removing MPI process constraints.
- **Matrix assembly** is parallelized to fit ScaLAPACK's **block-cyclic distribution**.
- **3-body solver**: replaces MKL routines with **ScaLAPACK's** parallel linear algebra routines.

These improvements **enhance performance** and **remove memory limitations**, enabling the handling of larger problems.



MPI profiling of the upgraded 2-body routine

With the **task-based distribution**, the imbalance is completely resolved and the time to solution is highly reduced.

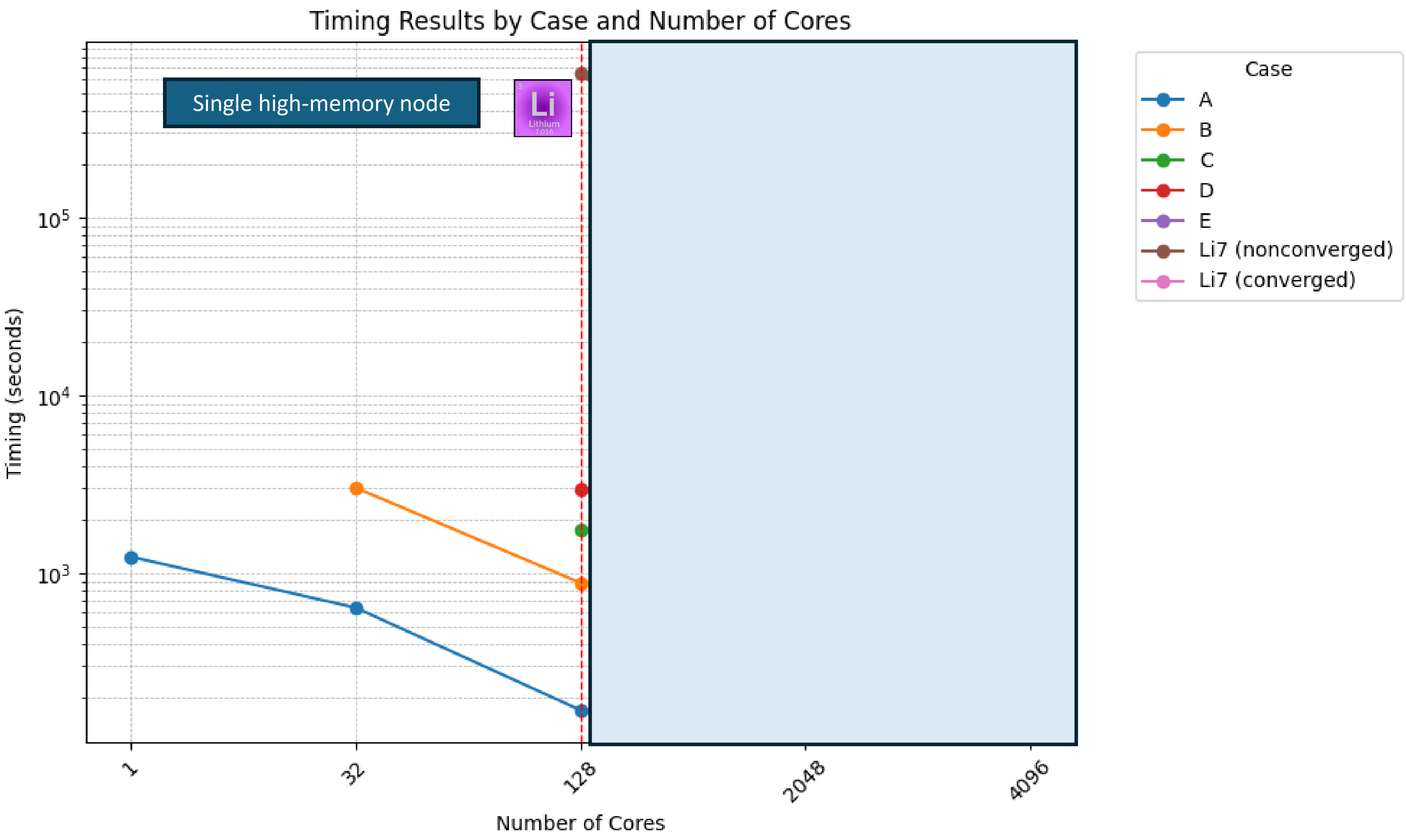


Overview of the upgraded full three-body quantum systems solver

Initially, physics were **constrained to the available memory** in a single, high-memory node.

- The Lithium few-body puzzle could be solved, but **not completely converged**.

The simulation time was several days, necessitating **checkpointing and restarting.**

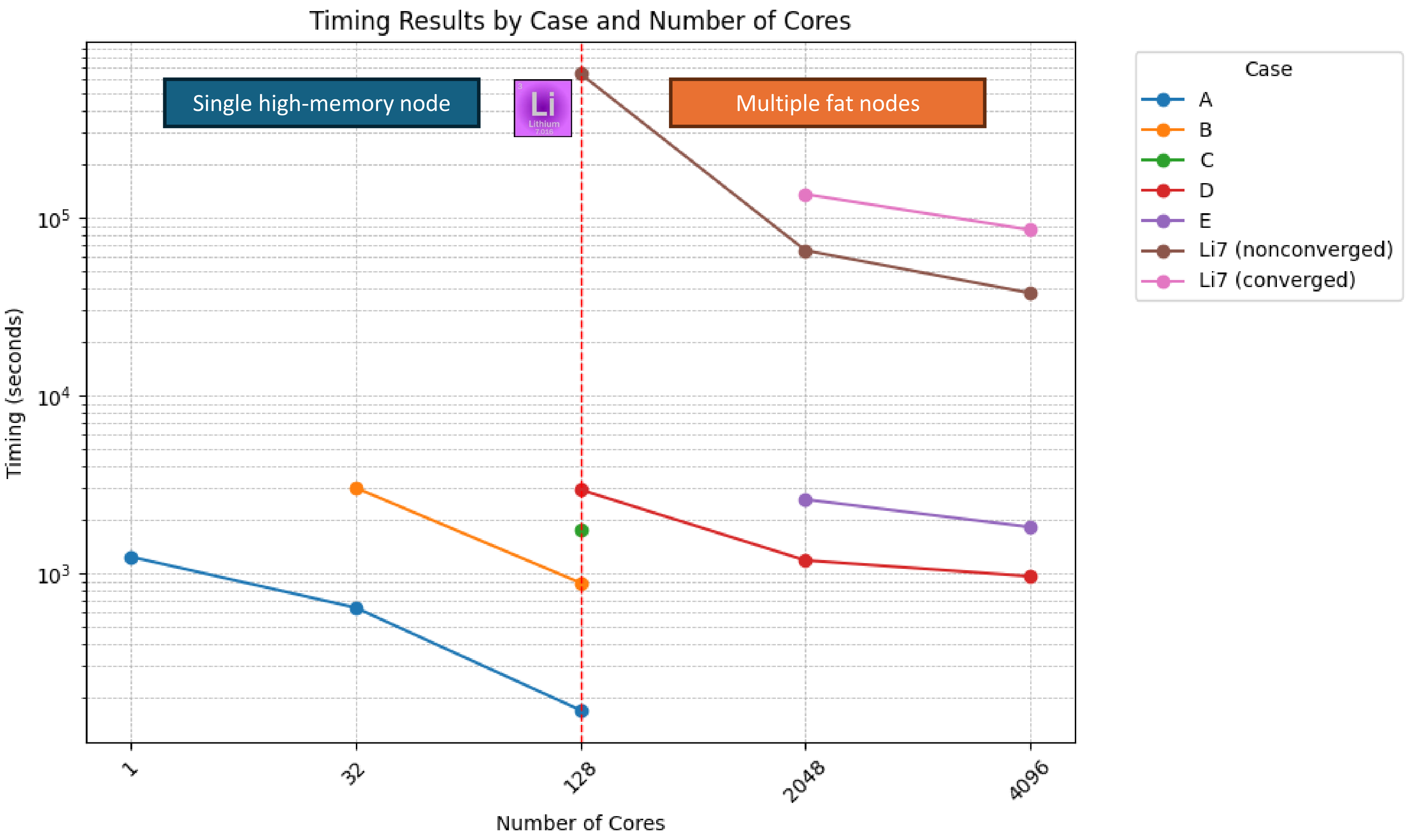


Overview of the upgraded full three-body quantum systems solver

The fully distributed, task-based implementation allows to **efficiently scale** on distributed parallel systems:

- **Memory constraint is broken.**
- **Wall-clock time is reduced.**

The upgraded implementation **enabled to solve more physics in fewer time.**



Thank you for listening!

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