Few-body physics with many processors

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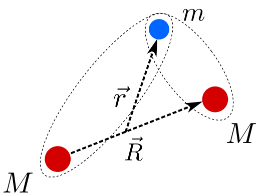
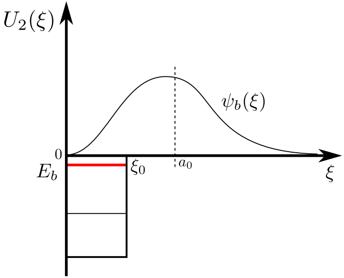
Quantum-mechanical three-body system



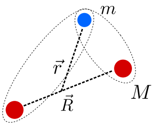
$$U\left(\vec{R},\vec{r}\right) = U_2\left(\left|\frac{\vec{R}}{2}+\vec{r}\right|\right) + U_2\left(\left|\frac{\vec{R}}{2}-\vec{r}\right|\right)$$



Goals:

- Obtain energies E_k and wave functions $\psi_k(\vec{R},\vec{r})$
- Investigate the universal regime for a resonant two-body interaction U_2 (independent of its nature and/or shape)
- Study the properties of the three-body system for different
  - dimensionality (1D, 2D or 3D)
  - mass ratio m/M
  - symmetry of two-body resonance (s-wave or p-wave)

Dimensionality and resonance symmetry



Symmetry of two-body resonance →

Dimension ↑

	s-wave resonance	p-wave resonance
3	$E_k \sim \exp(-\alpha k)$ $N_b = \infty$ $\mathcal{V}(R) \sim -\frac{1}{mR^2}$ *(Efimov effect)*	$E_k \sim -(k-k_*)^6$ $\mathcal{V}(R) \sim -\frac{1}{mR^3}$ $N_b < \infty$
2	$E_k \sim -\frac{1}{(k-\delta)^2}$ $N_b < \infty$ $\mathcal{V}(R) \sim -\frac{1}{mR}$ $\xi_0 \ll R \ll a_0^{(2)}$	1) $\ell = 0$: $E_k \sim ?$ 2) $\ell = \pm 1$: $E_k \sim \exp\left[-2\exp\left(2\pi \frac{m}{M} k + \theta\right)\right]$ $N_b = \infty$

[1] F.F. Bellotti et al., J. Phys. B: At.Mol.Opt.Phys. **46**, 055301 (2013)
[2] M.A. Efremov, L. Plimak, M. Yu. Ivanov, W.P. Schleich, PRL **111**, 113201 (2013)
[3] S. Moroz and Y. Nishida, PRA **90**, 063631 (2014)

Stationary three-body Schrödinger equation

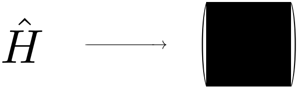
$$\underbrace{\left[-\frac{\hbar^2}{M}\Delta_{\vec{R}} - \frac{\hbar^2}{2\mu_2}\Delta_{\vec{r}} + U(\vec{R},\vec{r})\right]}_{\hat{H}} \psi_k\left(\vec{R},\vec{r}\right) = E_k \psi_k\left(\vec{R},\vec{r}\right)$$

$$\psi_k\left(\vec{R},\vec{r}\right)\Big|_{|\vec{R}|\to\infty,\,|\vec{r}|\to\infty} = 0$$

$\Rightarrow$ Obtain energies E_k and wave functions $\psi_k(\vec{R},\vec{r})$

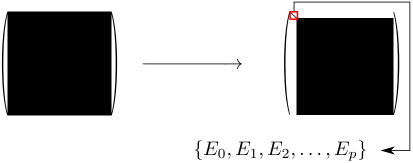
Numerical approach

1. **Discretization:** Obtain accurate, partial representation of the spectrum by a sufficient small matrix ($\geq 10^8 \times 10^8$)



$\Rightarrow$ **Spectral methods**

2. **Diagonalization:** Extract eigenvalues of interest

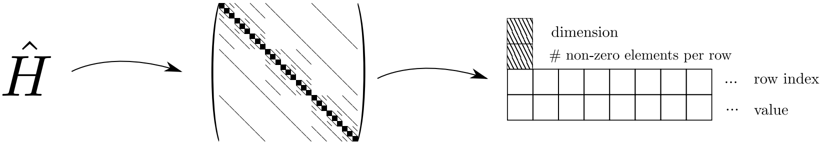


$\Rightarrow$ **Arnoldi iteration, Lanczos methods**

Implementation on the Data Vortex (example)

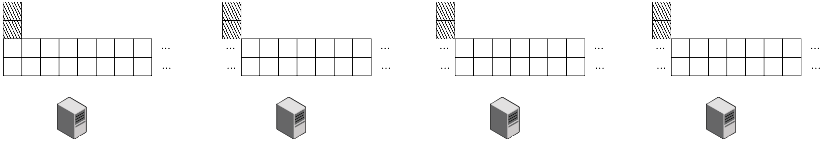
1. **Sparse matrix storage format**

   dim: Matrix dimension
   nz: Number of non-zero elements per row



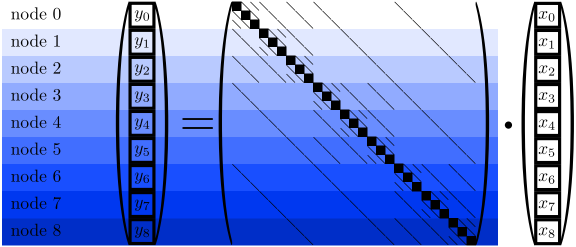
   $N = 100$: Matrix size $10^8 x 10^8 \approx 450$ GB

2. **Parallel (partial) matrix generation** (No communication)



Implementation on the Data Vortex

3. **Eigenvalue/-vector calculation**
   We implemented a parallel version of ARPACK (*Arnoldi iteration package*) using MPI on the DataVortex.
4. **Basic routine**: Parallelized matrix-vector product



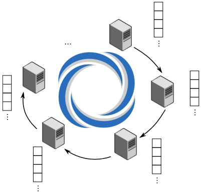
$$y = H^{(4)} \cdot x$$

Implementation on the Data Vortex

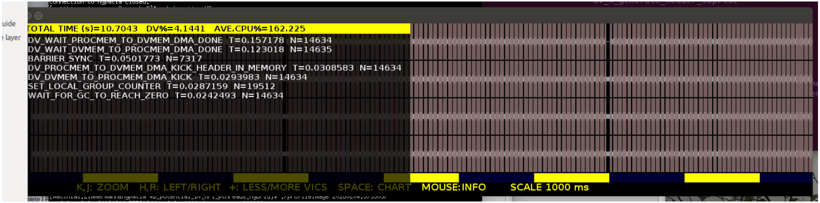
5. **Communication**

   Broadcast y_i to all nodes via the DV network

   Number of iterations: 10 000-500 000

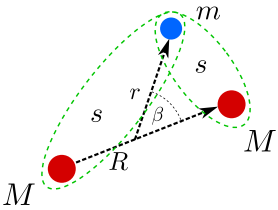


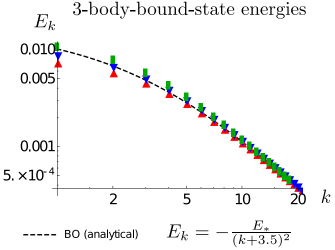
Analysis with Data Vortex profiler



Results for three particles in 2D: universal behaviour and *s*-wave resonance

$M/m = 10^4$





$E_b^s = 10^{-4}\frac{1}{\mu_2 \xi_0^2}$