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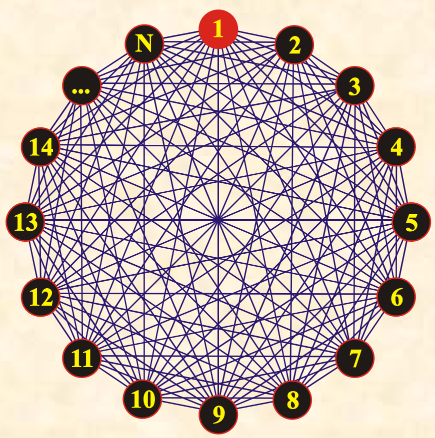
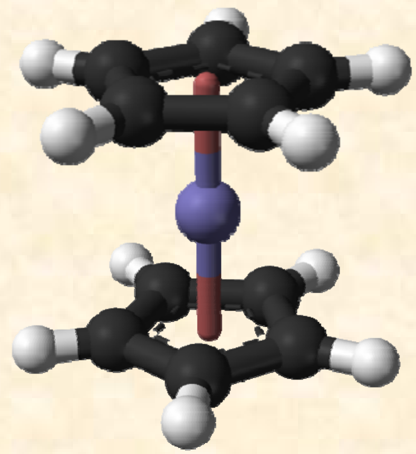
FAMAF Facultad de Matemática Astronomía y Física

GPU enhanced spin dynamics with Trotter-Suzuki evolutions





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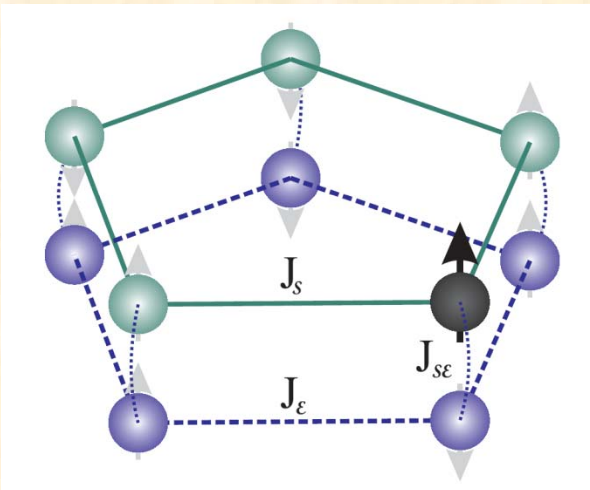
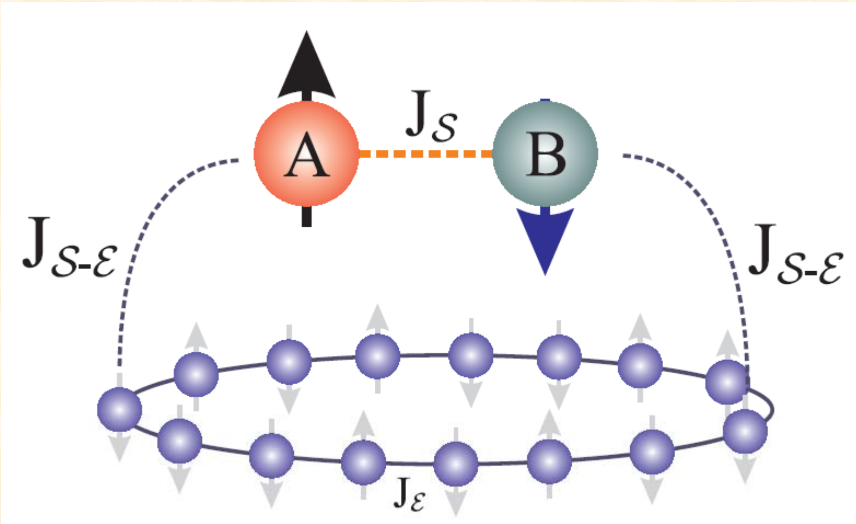
Spin Dynamics

Study Spin dynamics (with Many-Body interactions) using Trotter-Suzuki

Objective: Accelerate Quantum Spin Dynamics simulations.





$$\mathbf{U}(t) = e^{-\mathrm{i}tH}$$

$$H = \text{System Hamiltonian}$$

Trotter-Suzuki Approximation

$$\mathbf{U}(t) = e^{-\mathrm{i}tH} = e^{-\mathrm{i}t(H_1+...+H_K)} = \lim_{m\to\infty}\left(\prod_{k=1}^{K} e^{-\frac{\mathrm{i}tH_k}{m}}\right)^m$$

First order Approximation

$$\tilde{\mathbf{U}}_{\mathbf{1}}(t) = e^{-\mathrm{i}tH} = e^{-\frac{\mathrm{i}tH_1}{m}}...e^{-\frac{\mathrm{i}tH_K}{m}}$$

High orders Approximations

$$\tilde{\mathbf{U}}_{\mathbf{2}}(t) = \tilde{\mathbf{U}}_{\mathbf{1}}^{\dagger}(-t/2)\tilde{\mathbf{U}}_{\mathbf{1}}(t/2)$$

$$\tilde{\mathbf{U}}_{\mathbf{4}}(t) = \tilde{\mathbf{U}}_{\mathbf{2}}(at)\tilde{\mathbf{U}}_{\mathbf{2}}(at)\tilde{\mathbf{U}}_{\mathbf{2}}((1-4a)t)\tilde{\mathbf{U}}_{\mathbf{2}}(at)\tilde{\mathbf{U}}_{\mathbf{2}}(at)$$

$$a = 1/(4-4^{1/3})$$

H. De Raedt and K. Michielsen, Handbook of Theoretical and Computational Nanotechnology (American Scientific Publishers)

Trotter-Suzuki Approximation

Many-Body spin Hamiltonian

$$H = \sum_{j=1}^{N} \sum_{\alpha=x,y,z} h_j^\alpha \; S_j^\alpha + \sum_{j,k=1}^{N} \sum_{\alpha=x,y,z} J_{j,k}^\alpha S_j^\alpha S_k^\alpha$$

Single Spin Operators

$$\exp\left(-\mathrm{i}t\left[\sum_{j=1}^{N} \sum_{\alpha=x,y,z} h_j^\alpha \; S_j^\alpha\right]\right) = \prod_{j=1}^{N} \exp\left(-\mathrm{i}t \sum_{\alpha=x,y,z} h_j^\alpha \; S_j^\alpha\right)$$

Trotter-Suzuki Approximation

Two spin Operators

$$H^z = \sum_{j,k=1}^{N} J^z_{j,k} S^z_j S^z_k$$

It only modify the phase of each states (trivial parallelization)

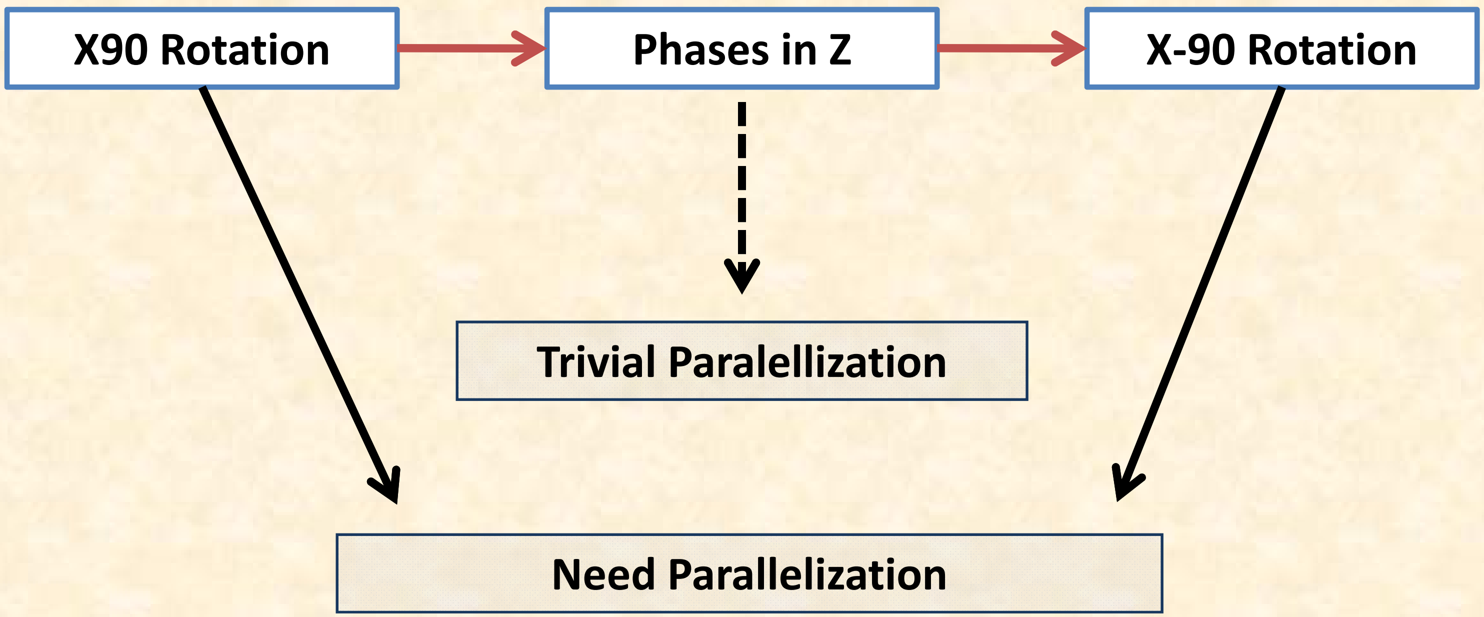
Using Rotations we can rewrite H^x y H^y

$$Y = \prod_{j=1}^{N} Y_j \qquad e^{-\mathrm{i}tH^x} = \bar{Y} Y e^{-\mathrm{i}tH^x} \bar{Y} Y = \bar{Y} \exp\left(-\mathrm{i}t \left[\sum_{j,k=1}^{N} J^x_{j,k} S^z_j S^z_k\right]\right) Y$$

$$X = \prod_{j=1}^{N} X_j \qquad e^{-\mathrm{i}tH^y} = X \bar{X} e^{-\mathrm{i}tH^y} X \bar{X} = X \exp\left(-\mathrm{i}t \left[\sum_{j,k=1}^{N} J^y_{j,k} S^z_j S^z_k\right]\right) \bar{X}$$

Trotter-Suzuki Algorithm

Two spin Operators

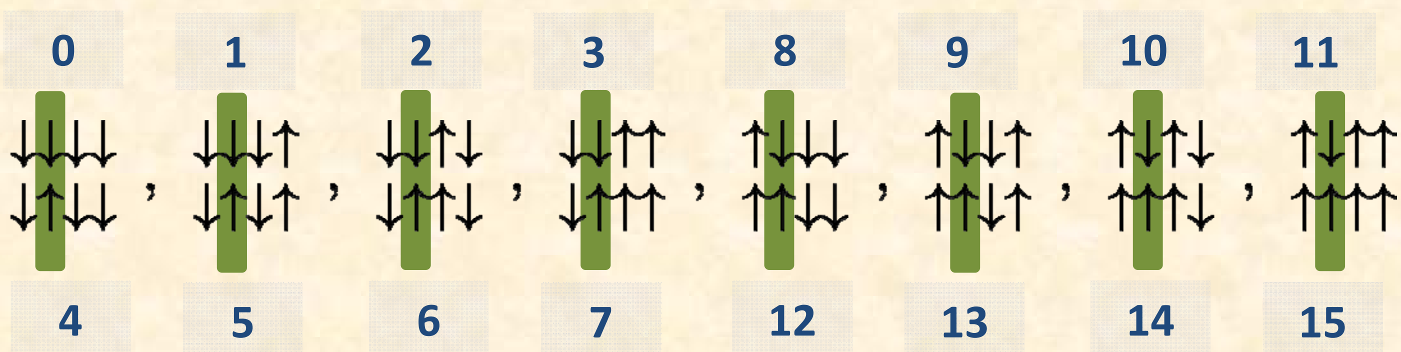


Trotter-Suzuki Algorithm

Rotations

$$X = \prod_{j=1}^{N} X_j \longrightarrow \exp\left(-itS_j^{\alpha}\right)$$

N=4 Spins and select j=2



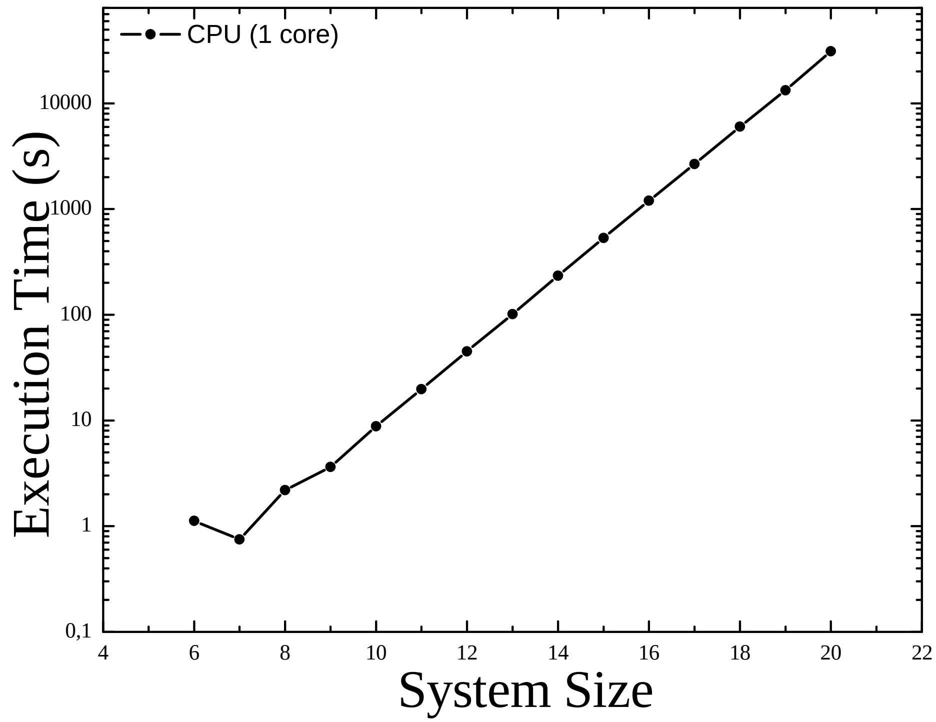
Individual Rotations are Parallelizable

GPU implementation

Intel DX58SO motherboard with
Intel Core i7-950 3.07GHz 16GB DDR3 1066MHz,

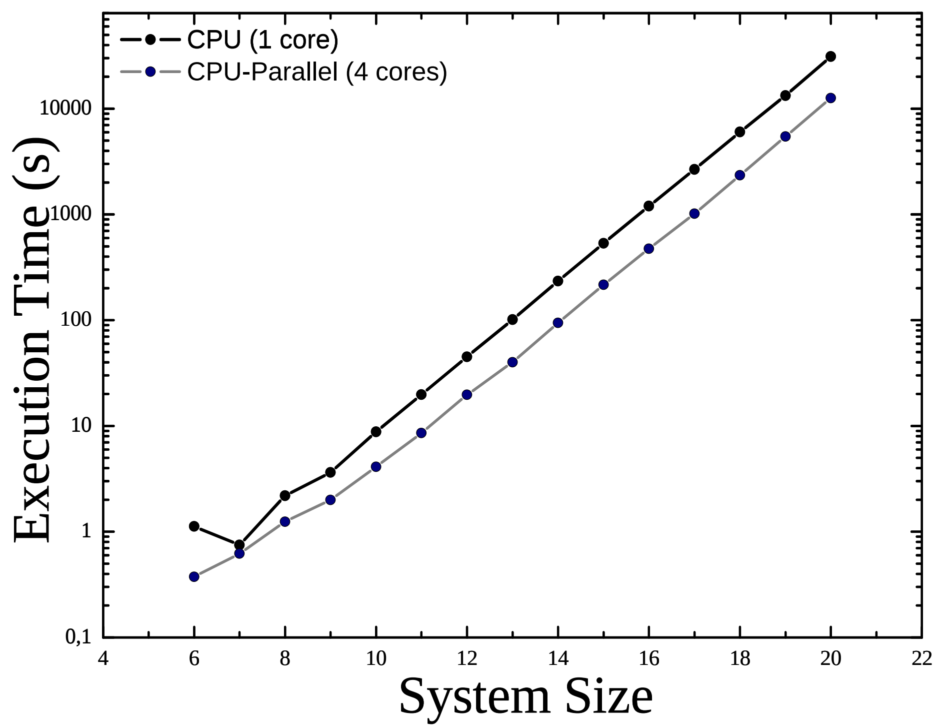
twoTesla C2070 boards
(448 cores, 6GB GDDR5),
donated by NVIDIA.

CPU vs GPU



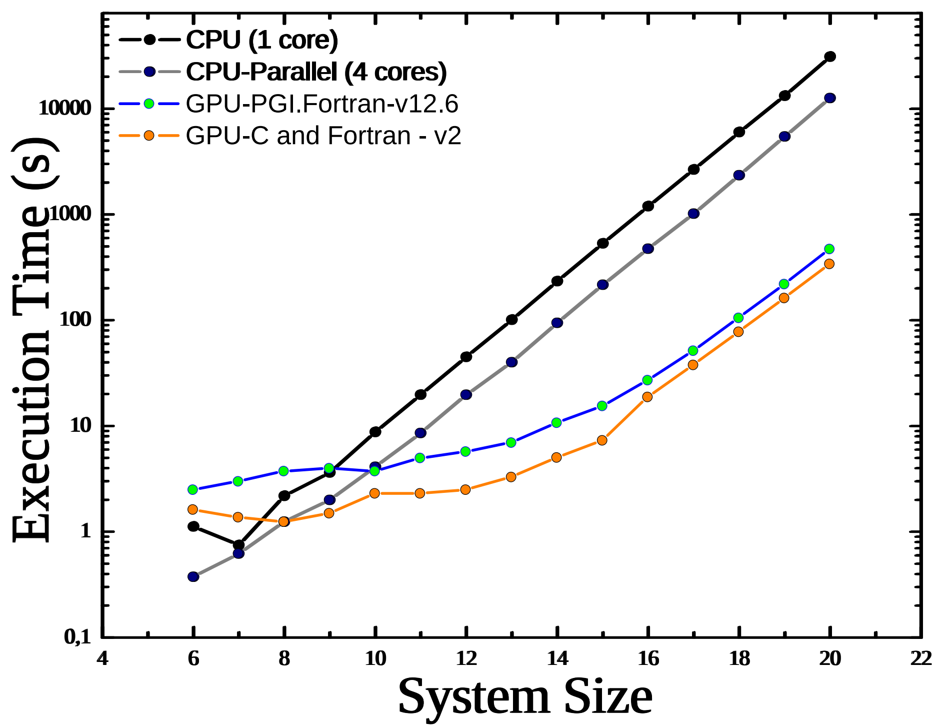
Max of 28 Spins in one GPU (limited by the GPU memory)

CPU vs GPU



Max of 28 Spins in one GPU (limited by the GPU memory)

CPU vs GPU



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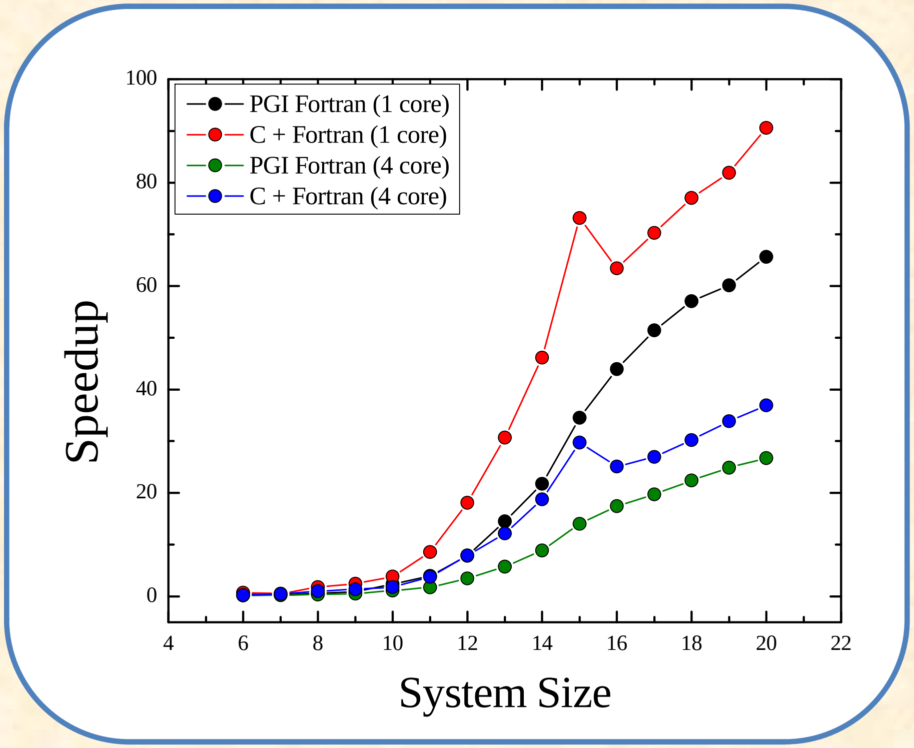
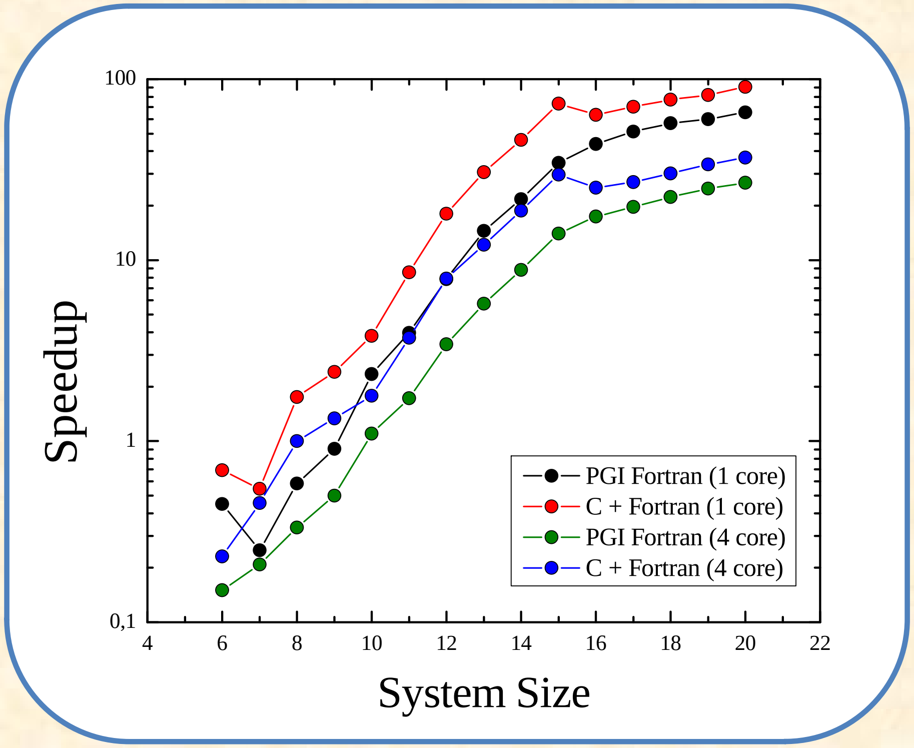
CPU vs GPU



PGI Fortran (1 core)
C + Fortran (1 core)
PGI Fortran (4 core)
C + Fortran (4 core)
Speedup
System Size



PGI Fortran (1 core)
C + Fortran (1 core)
PGI Fortran (4 core)
C + Fortran (4 core)
Speedup
System Size

Conclusions

Parallelized the Trotter-Suzuki CPU algorithm for spin dynamics and implement it on GPUs.

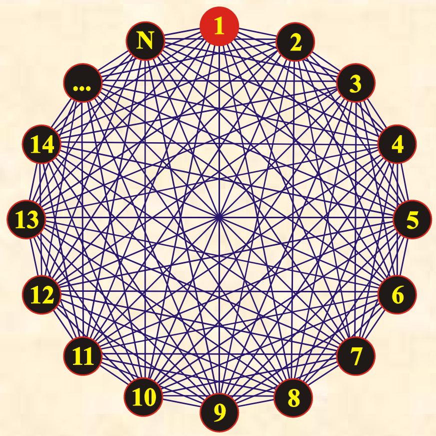
Compared TWO compilers (Fortran and C)

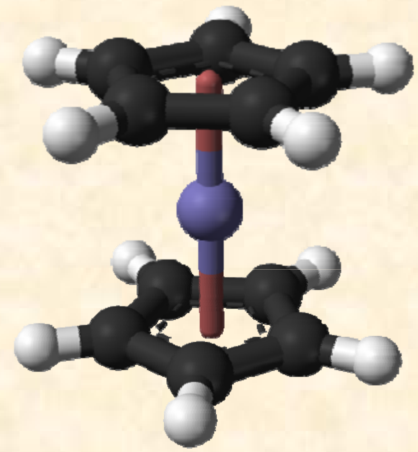
Obtain a maximum Speedup of 90x (compared with a single core) and 36x (compared with 4 cores)

Perspectives

Develop a new code based on this algorithm for NMR simulations

Questions?





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