# In-medium no-core shell model

## An *ab initio* path towards medium-mass nuclei

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# Outline

- No-core shell model and its limitations
- In-medium similarity renormalization group
- Results on $^{12}C$ and $^{20}O$
- Outlook

# No-core shell model

- Transform stationary Schrödinger equation

$$H |\psi_n\rangle = E_n |\psi_n\rangle$$

into matrix eigenvalue problem inserting a spherical basis of HO Slater determinants

$$\sum_j \langle\phi_i| H |\phi_j\rangle \langle\phi_j|\psi_n\rangle = E_n \langle\phi_i|\psi_n\rangle \quad \forall i$$

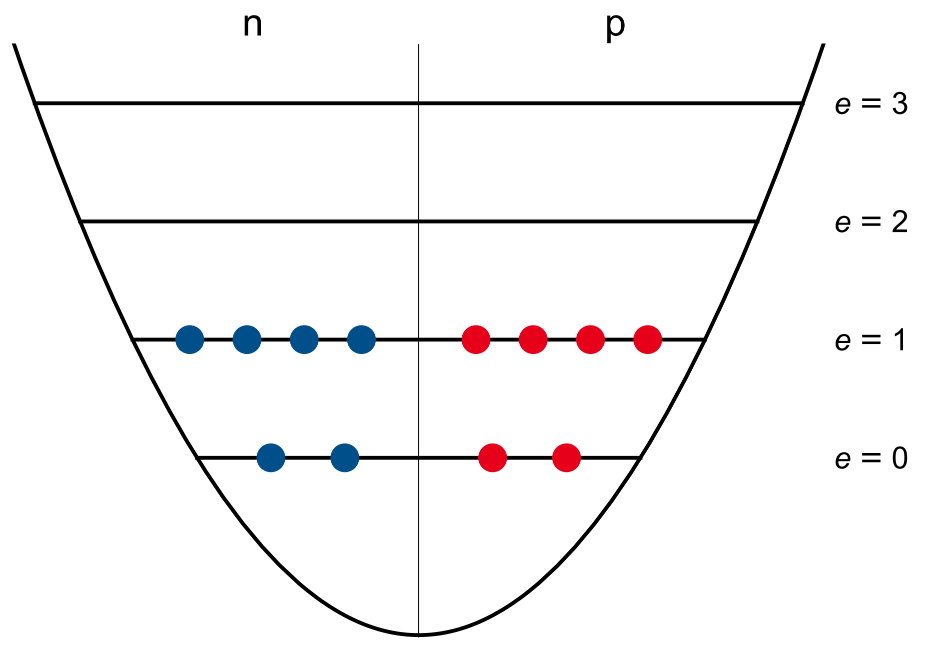
$$\begin{pmatrix} \langle\phi_1|H|\phi_1\rangle & \langle\phi_1|H|\phi_2\rangle & \langle\phi_1|H|\phi_3\rangle & \cdots \\ \langle\phi_2|H|\phi_1\rangle & \langle\phi_2|H|\phi_2\rangle & \langle\phi_2|H|\phi_3\rangle & \cdots \\ \langle\phi_3|H|\phi_1\rangle & \langle\phi_3|H|\phi_2\rangle & \langle\phi_3|H|\phi_3\rangle & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \langle\phi_1|\psi_n\rangle \\ \langle\phi_2|\psi_n\rangle \\ \langle\phi_3|\psi_n\rangle \\ \vdots \end{pmatrix} = E_n \begin{pmatrix} \langle\phi_1|\psi_n\rangle \\ \langle\phi_2|\psi_n\rangle \\ \langle\phi_3|\psi_n\rangle \\ \vdots \end{pmatrix}$$

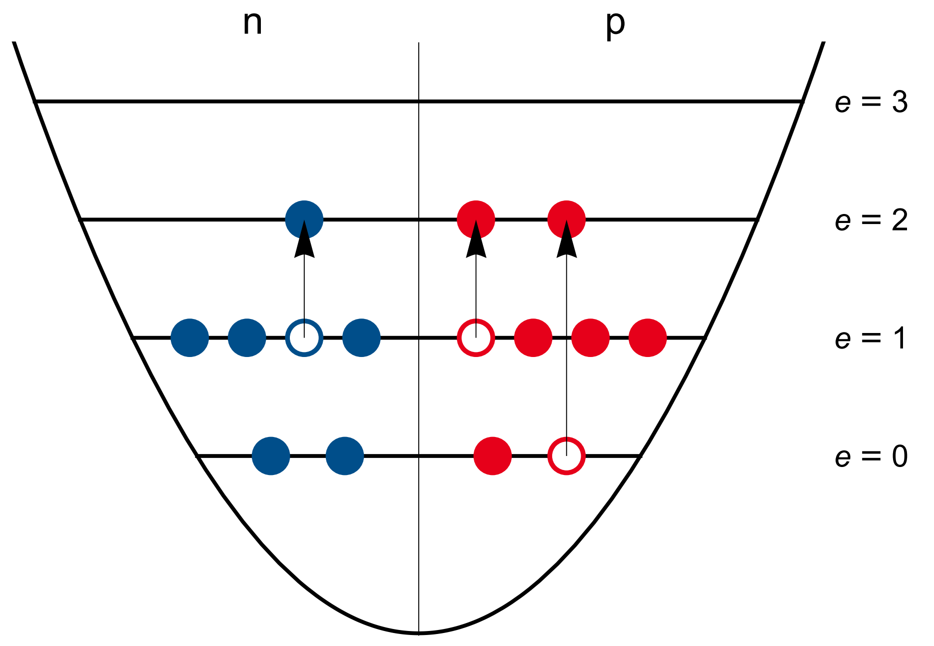
# $N_{\text{max}}$ truncation

- Truncation is needed to obtain finite problem
- Truncate in form of total number of HO excitation quanta $N_{\text{max}}$: $E_* - E_0 \leq N_{\text{max}} \hbar\Omega$
- Recover full Hilbert space with $N_{\text{max}} \to \infty$
- Model space space dimension grows combinatorically in $A$ and $N_{\text{max}}$
- NCSM only feasible for light nuclei

$^{12}$C

$N = 0$

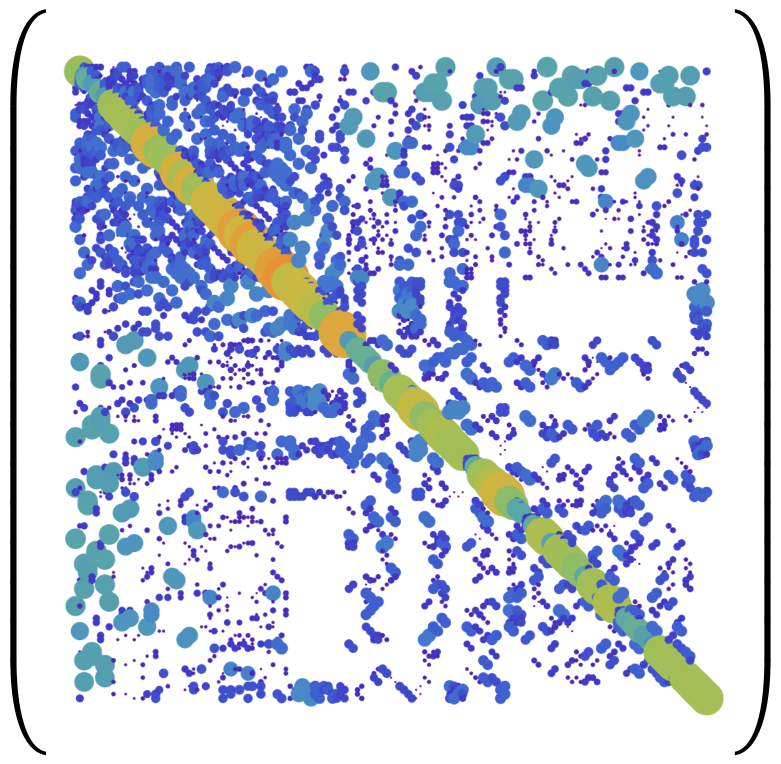



$N = 4$

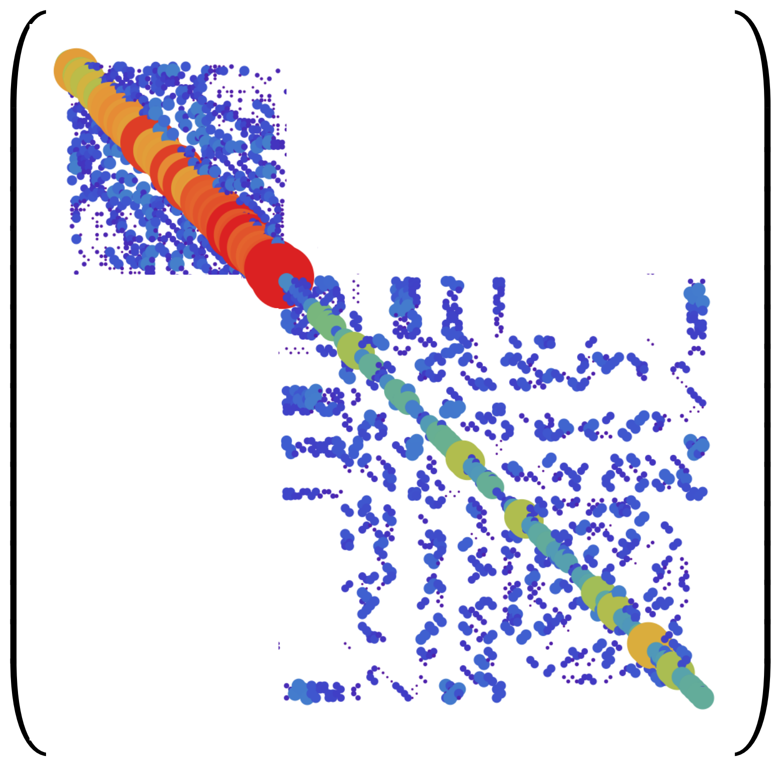
# Schematic $^{12}$C Hamiltonian matrix

- Hamiltonian matrix initially fully occupied
- Need large model space / $N_{\mathrm{max}}$



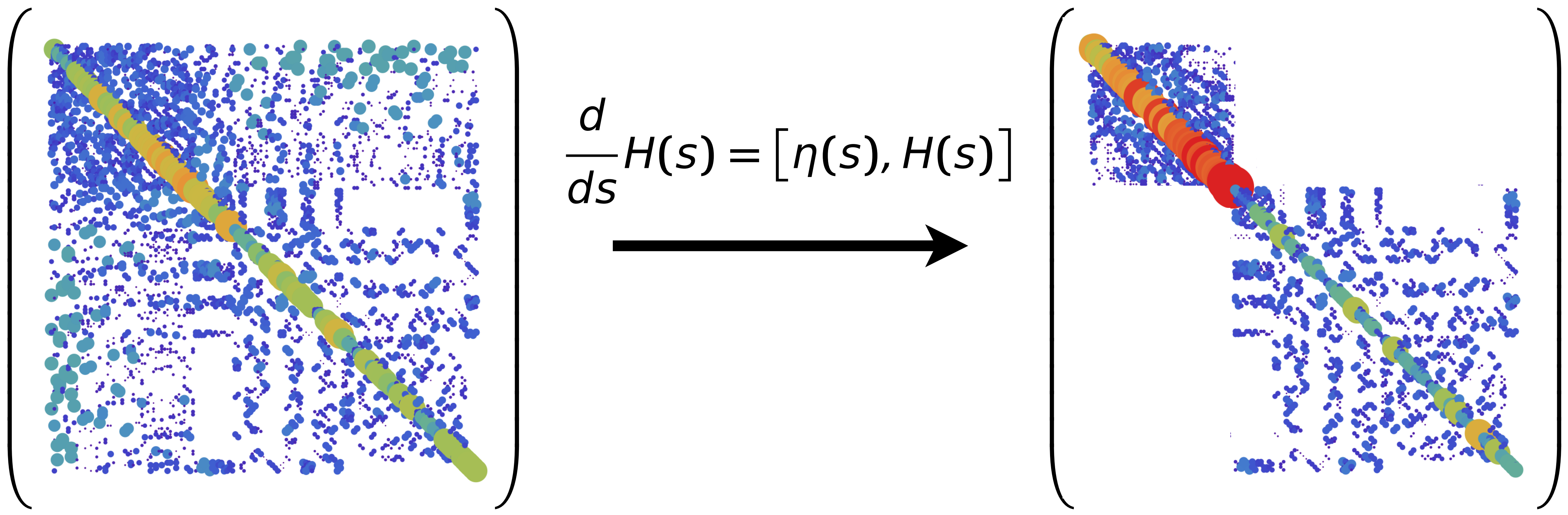
Courtesy of R. Roth

- More advantageous structure
- Fewer correlations in higher excitations
- Faster convergence in $N_{\mathrm{max}}$



# In-medium similarity renormalization group

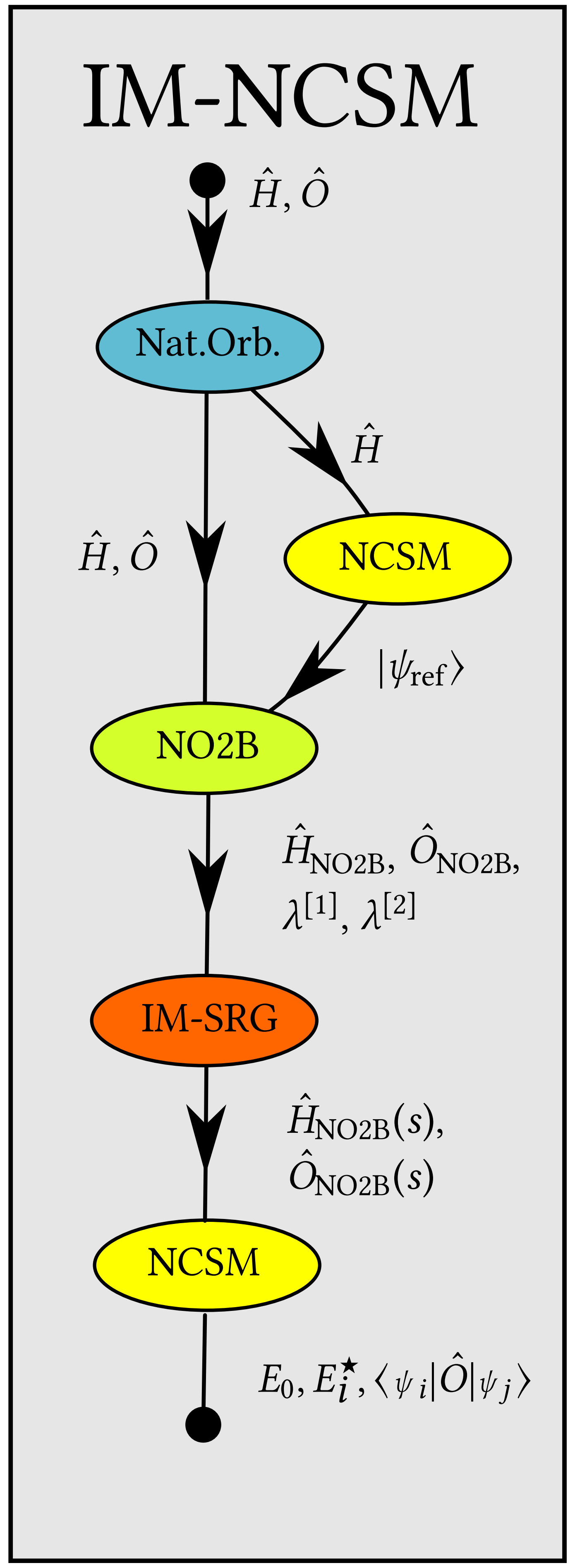
- Apply unitary transformation to Hamiltonian $H(s) = U^\dagger(s)H(0)U(s)$
- Carried out by the flow equation $\frac{\mathrm{d}}{\mathrm{d}s}H(s) = [\eta(s), H(s)]$
- Suppress „off-diagonal“ part of Hamiltonian with increasing *s*
- Final Hamiltonian in block diagonal/advantageous form



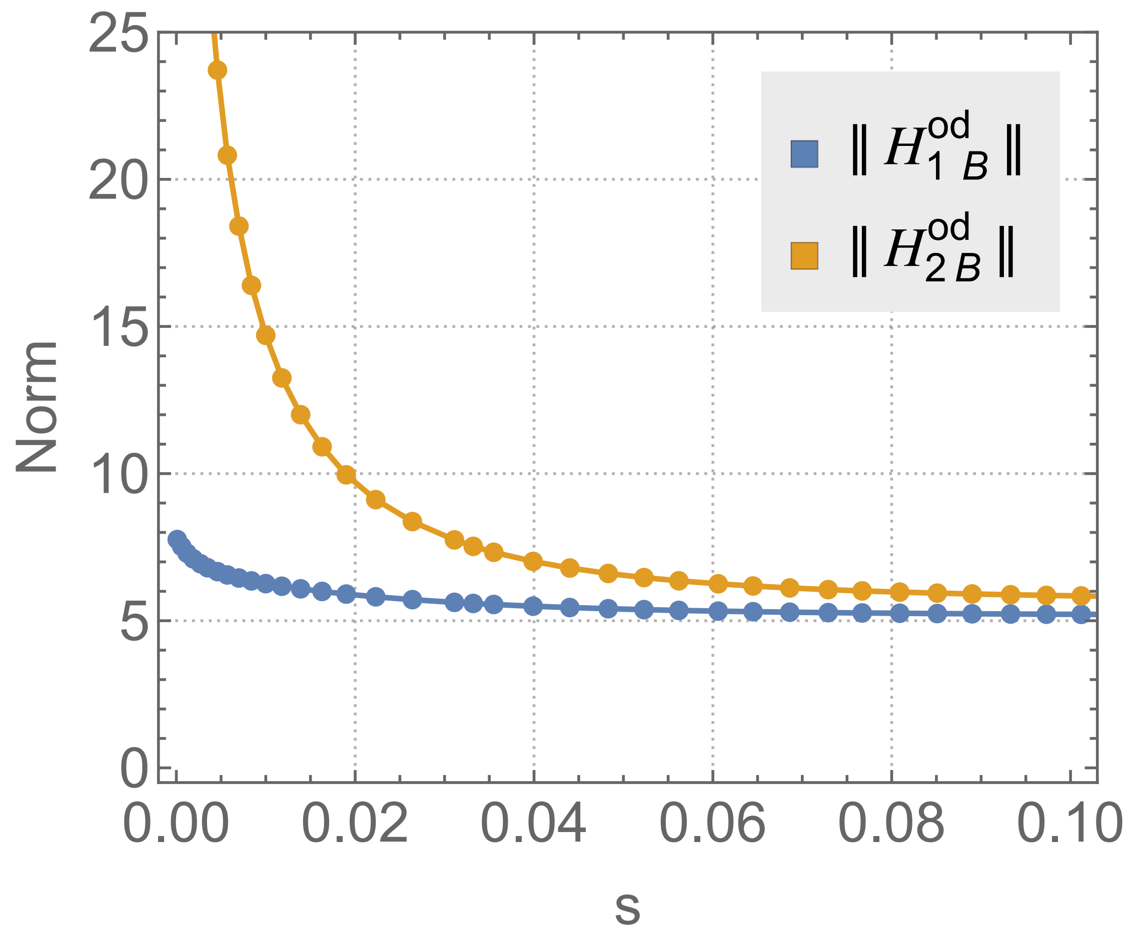
# In-medium no-core shell model

## *Ab initio* in medium-mass nuclei

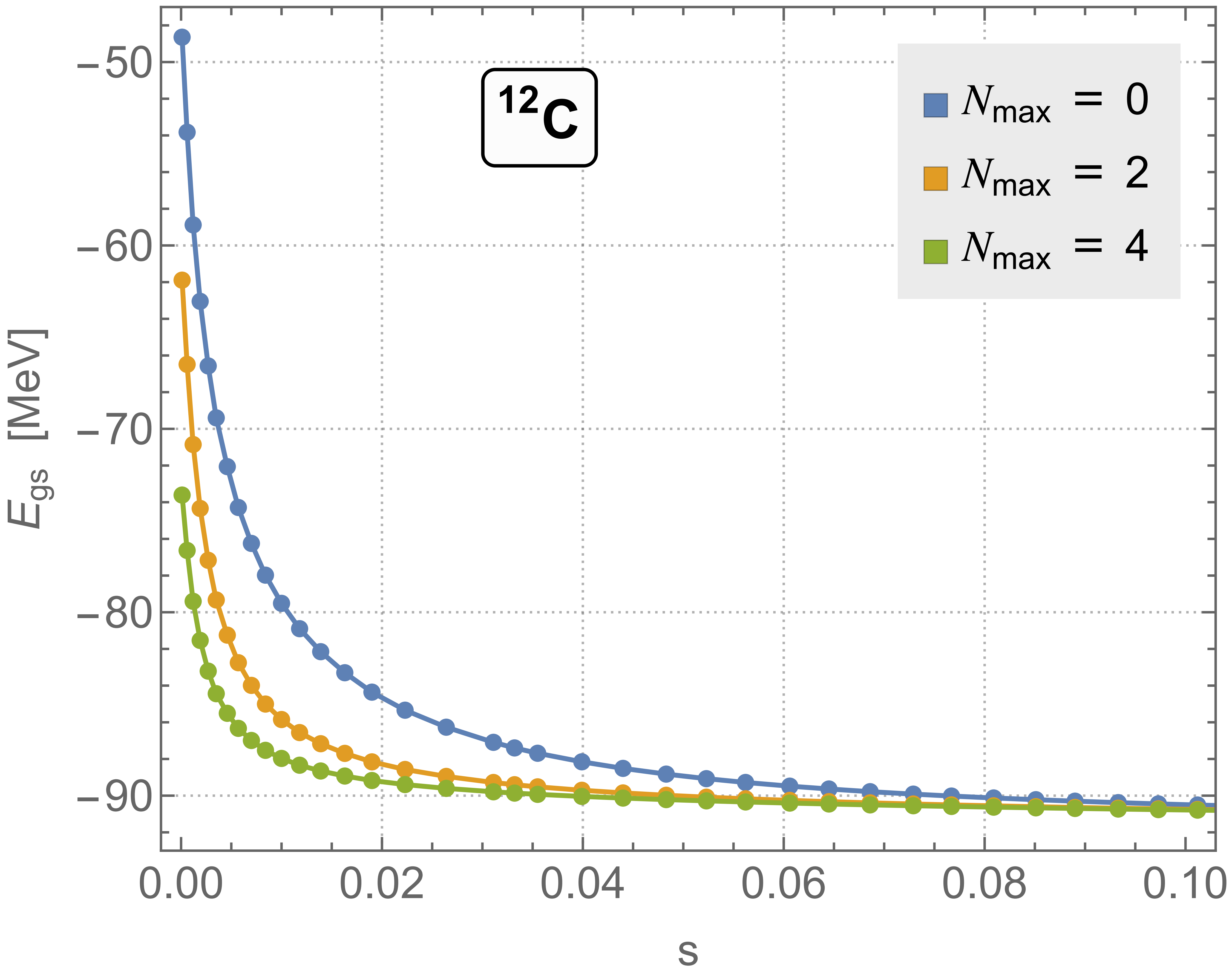
- Construct basis using natural orbitals
- Perform first, small NCSM computation to obtain reference state
- Run IM-SRG to decouple many-body Hilbert space
- Final NCSM diagonalization is sufficient in small model space
- Truncation uncertainties are trade off for convergence



# Ground-state energy flow $^{12}C$




- Perform NCSM diagonalization at intermediate flow parameters
- IM-SRG massively accelerates NCSM convergence
- Acceleration directly corresponds to suppression of off-diagonal part of Hamiltonian



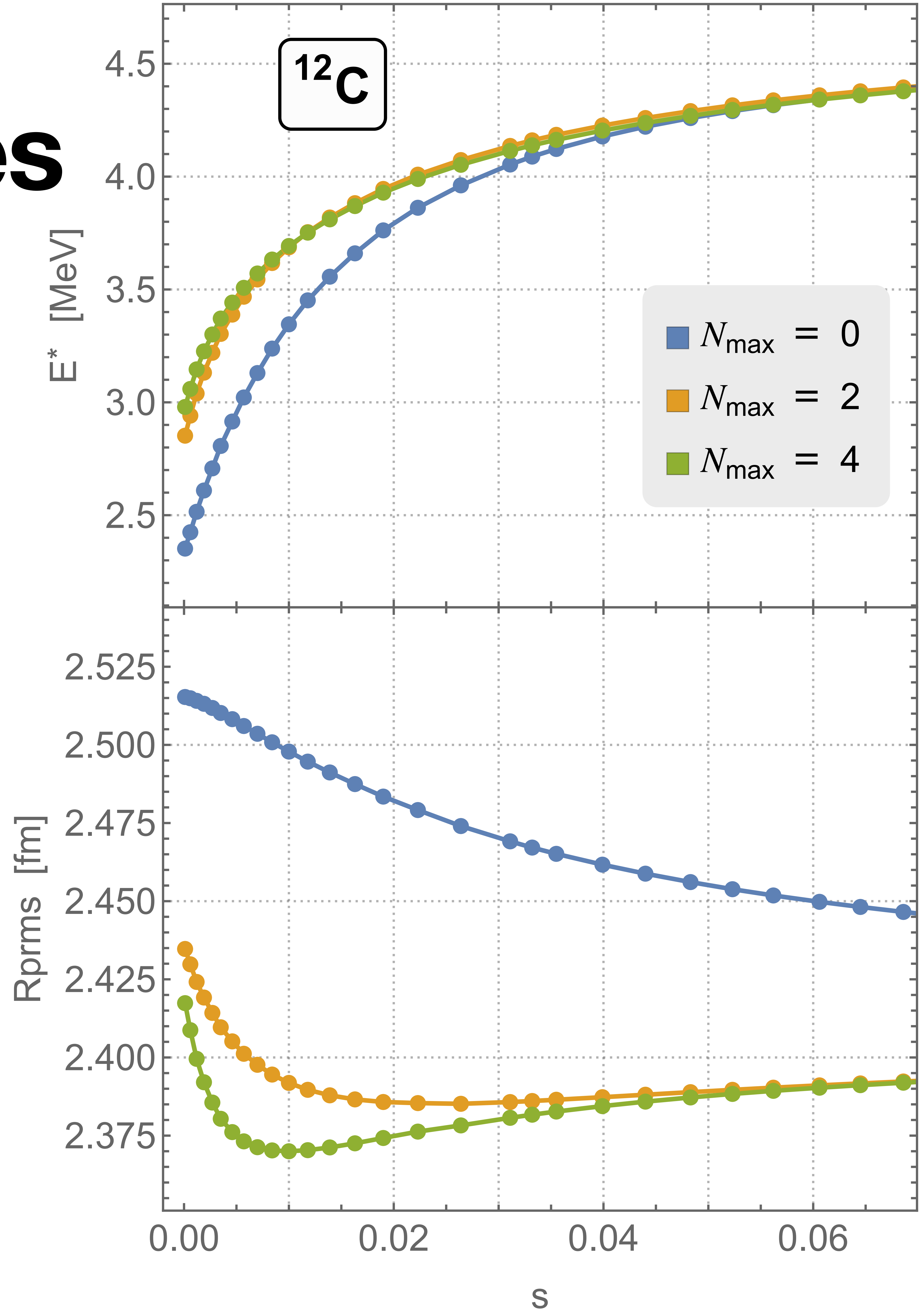
# Non-g.s.-energy observables

## Radius and 2+ excitation-energy

- IM-NCSM applicable to compute several observables

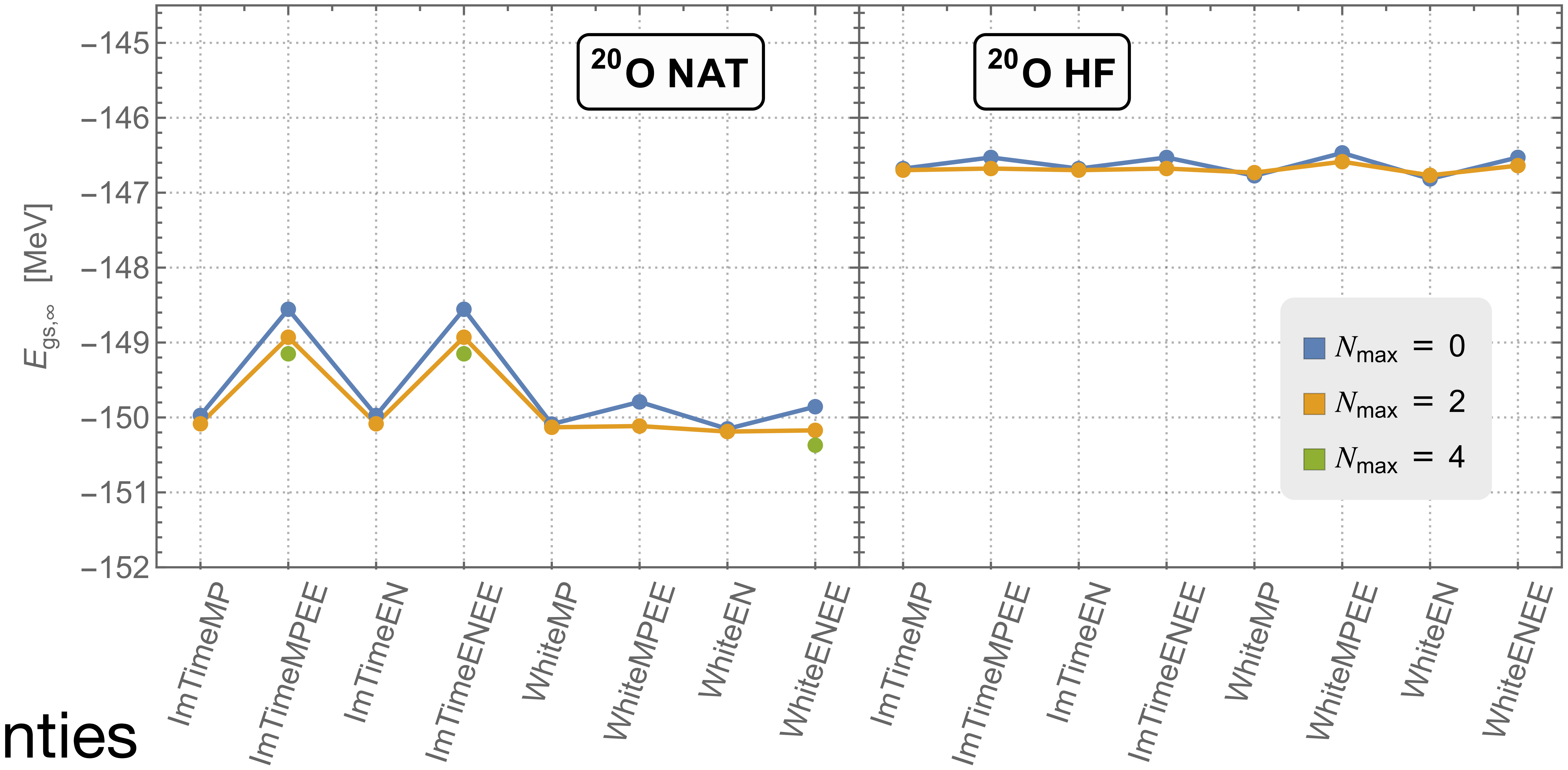
- Converge faster than g.s. energy

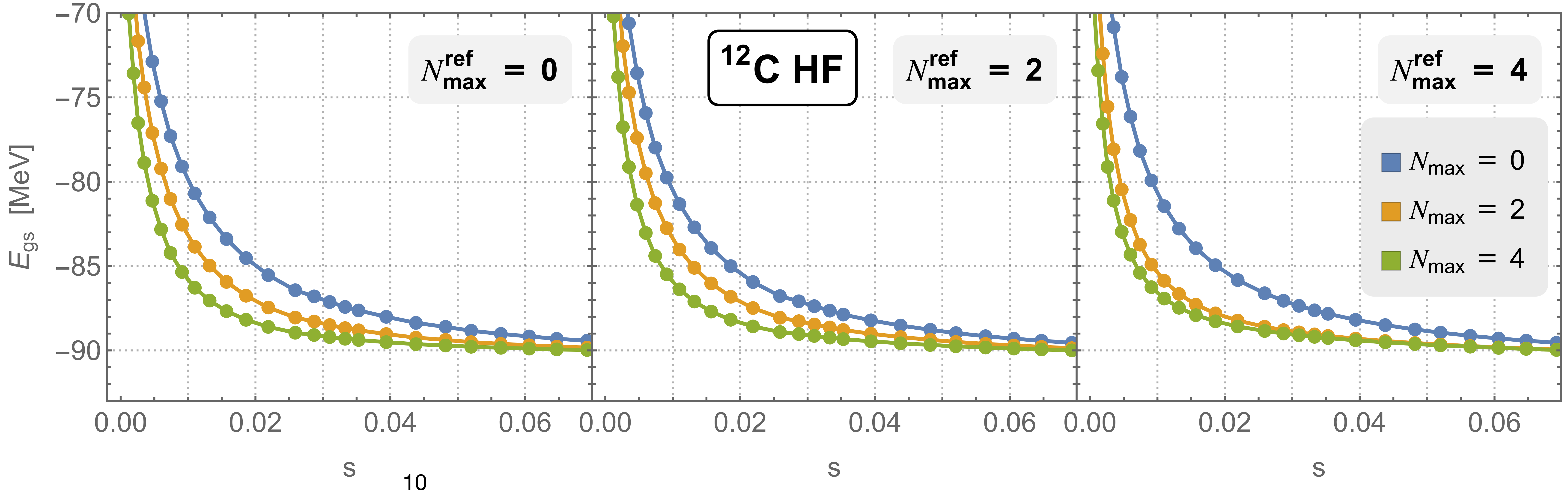
- $s_\infty$ determined by $E_{\text{g.s.}}$ flow



# Outlook

- Derive method uncertainty
- Find best balance between accuracy and numerical efficiency
- Reduce truncation uncertainties to minimum




- Thank you!!

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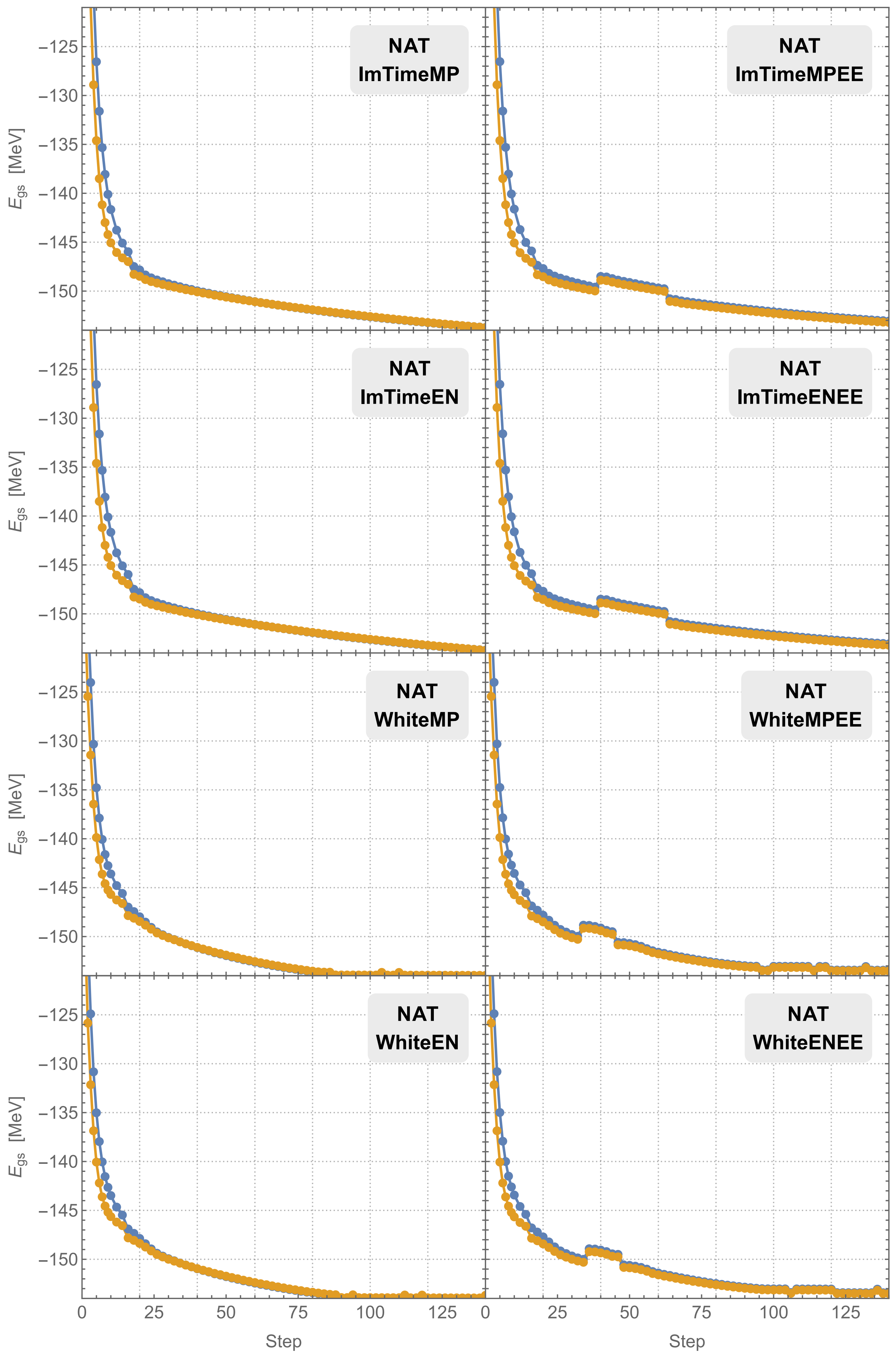
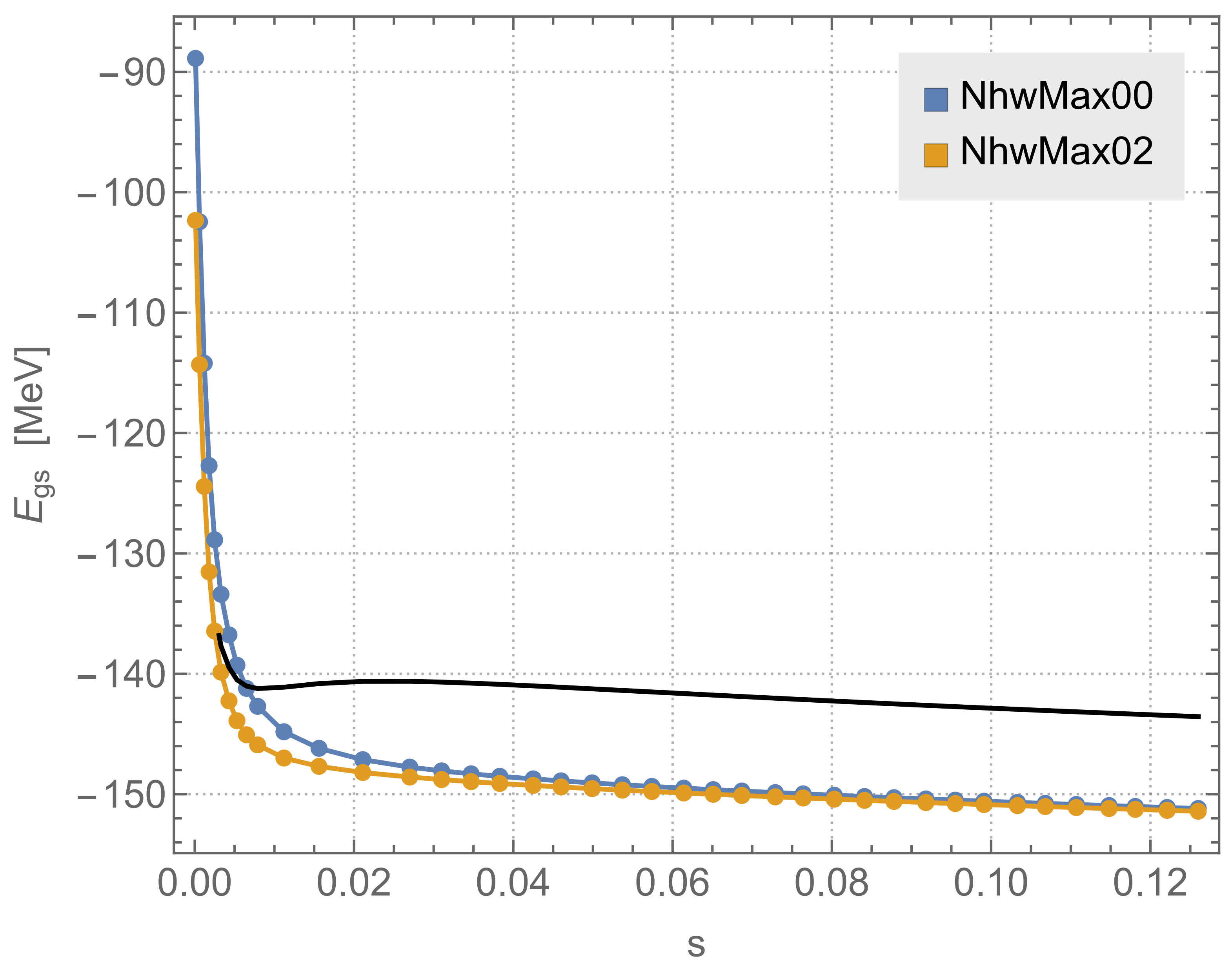
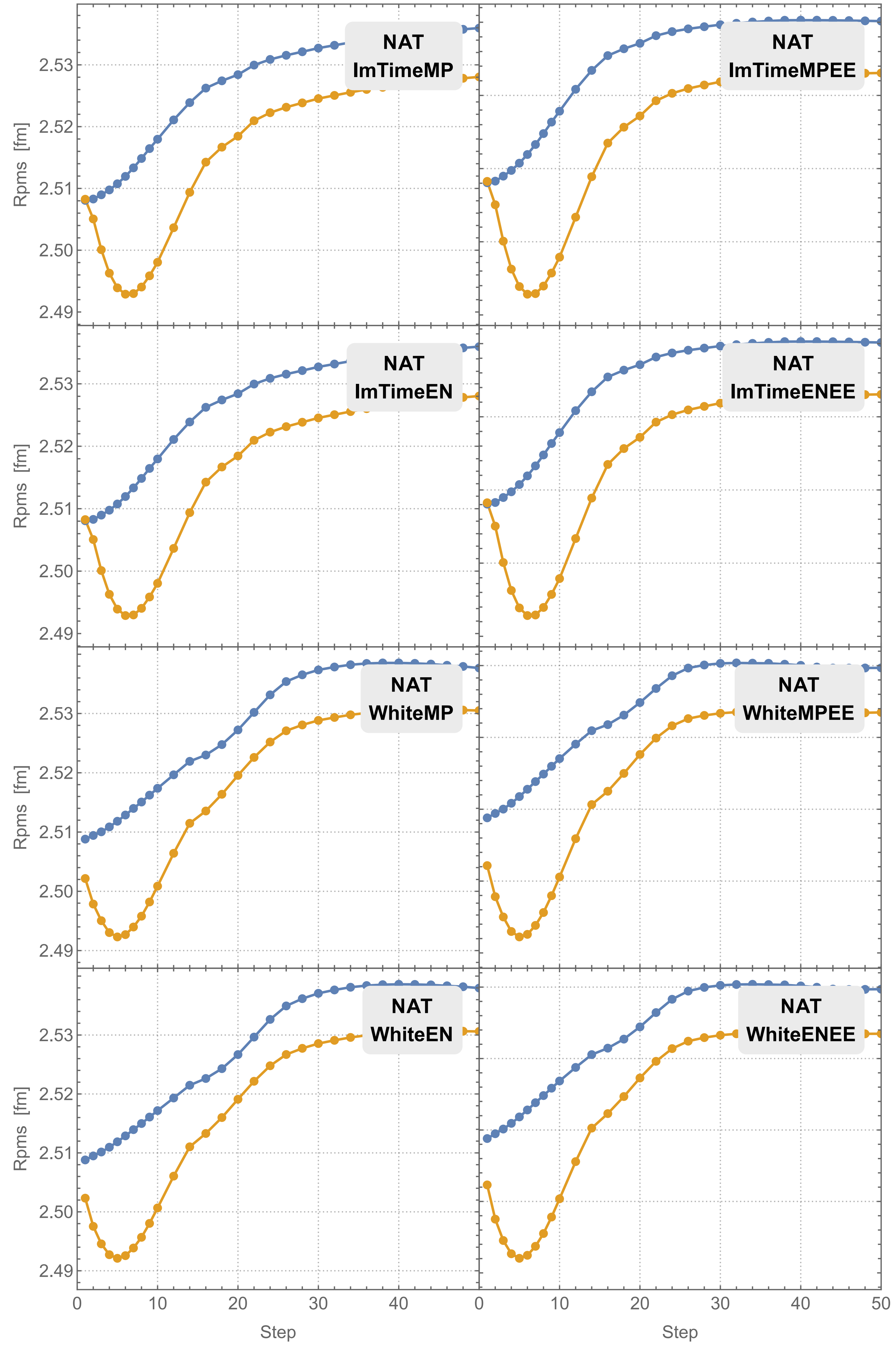
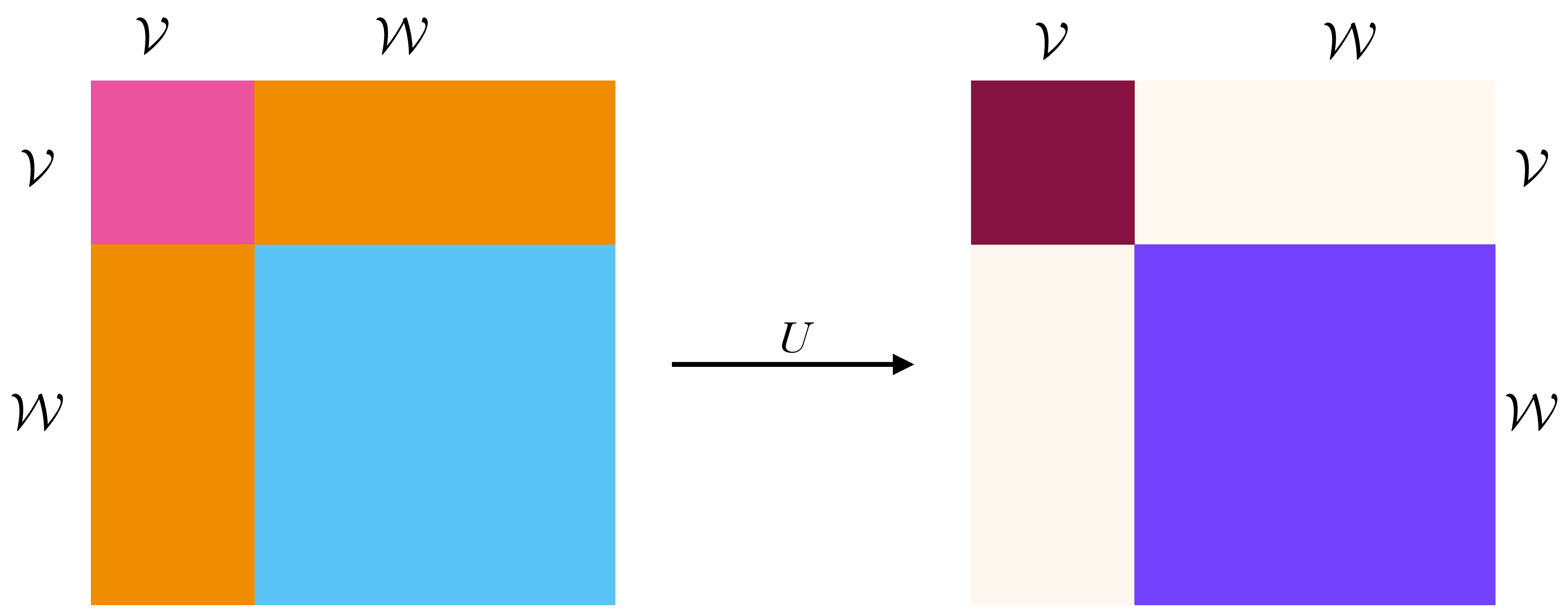
# Flow evolution - generator comparison



# Why is this advantageous?




- If $\mathcal{V} = \{|\psi_{\text{ref}}\rangle\}$: Schrödinger equation is solved via IM-SRG transformation
- For higher dimensional $\mathcal{V}$: Less information in higher excitations $\Longrightarrow$ Faster convergence
- Example: $\mathcal{V}$ is $N_{\text{max}}^{\text{ref}} = 2$ space, fewer correlation are carried in $N_{\text{max}} = 4, 6, ...$ space

# Normal ordering

$$a^{p_1 p_2 \dots p_n}_{q_1 q_2 \dots q_n} \equiv a^{p_1} a^{p_2} \dots a^{p_n} a_{q_n} \dots a_{q_2} a_{q_1}$$

$$\langle \psi_{\mathrm{ref}} | \, a^{p_1 p_2 \dots p_n}_{q_1 q_2 \dots q_n} \, | \psi_{\mathrm{ref}} \rangle \equiv \gamma^{p_1 p_2 \dots p_n}_{q_1 q_2 \dots q_n}$$

- Permute creation/annihilation operators s.t. their expectation value w.r.t reference state vanishes $\langle \psi_{\mathrm{ref}} | \left\{ a^{p_1 p_2 \dots p_n}_{q_1 q_2 \dots q_n} \right\} | \psi_{\mathrm{ref}} \rangle = 0$
- Wick's theorem links operators with its normal-ordered counterpart via contractions
- Information of higher particle ranks is stored into lower rank part of operators

$$X = V_0 + \sum_{pq} V^p_q a^p_q + \frac{1}{4} \sum_{pqrs} V^{pq}_{rs} a^{pq}_{rs} + \frac{1}{36} \sum_{pqrstu} V^{pqr}_{stu} a^{pqr}_{stu}$$

$$X = R_0 + \sum_{pq} R^p_q \{a^p_q\}_{|\psi_{\mathrm{ref}}\rangle} + \frac{1}{4} \sum_{pqrs} R^{pq}_{rs} \{a^{pq}_{rs}\}_{|\psi_{\mathrm{ref}}\rangle} + \frac{1}{36} \sum_{pqrstu} R^{pqr}_{stu} \{a^{pqr}_{stu}\}_{|\psi_{\mathrm{ref}}\rangle}$$

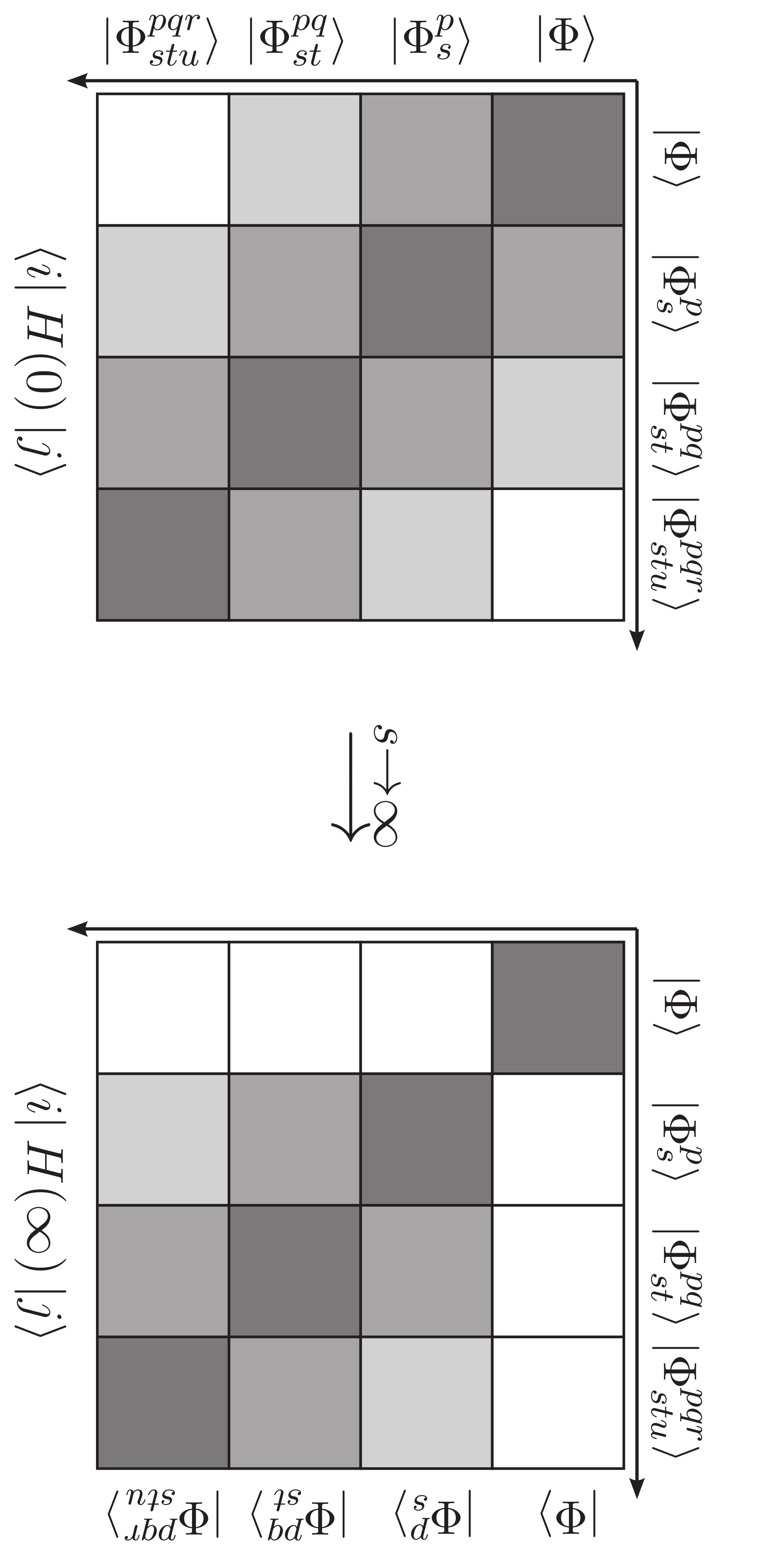
$$R_0 = V_0 + \sum_{pq} V^p_q \gamma^p_q + \frac{1}{4} \sum_{pqrs} V^{pq}_{rs} \gamma^{pq}_{rs} + \frac{1}{36} \sum_{pqrstu} V^{pqr}_{stu} \gamma^{pqr}_{stu}$$

$$R^1_2 = V^1_2 + \sum_{pq} V^{1p}_{2q} \gamma^{1p}_{2q} + \frac{1}{4} \sum_{pqrs} V^{1pq}_{2rs} \gamma^{pq}_{rs}$$

- Normal-Ordered Two-Body approximation (NO2B)

# Approaching equations of IM-SRG

## Particle-hole picture and flow equation




- Decouple reference state from its particle-hole excitations

$$\langle\psi_{\text{ref}}|H\{a^p_h\}|\psi_{\text{ref}}\rangle = f^p_h\overline{n}_p n_h \overset{!}{=} 0$$

$$H(s) \equiv U^\dagger(s)H(0)U(s) \iff \frac{\mathrm{d}}{\mathrm{d}s}H(s) = [\eta(s), H(s)]$$

- Various sophisticated generators available

- Magnus approach for evolution of multiple observables

$$U(s) = \exp(-\Omega(s))$$

$$\frac{\mathrm{d}}{\mathrm{d}s}\Omega(s) = \sum_{k=0}^{\infty}\frac{B_k}{k!}[\Omega(s), \eta(s)]_k \qquad O(s) = \sum_{k=0}^{\infty}\frac{1}{k!}[\Omega(s), O(0)]_k$$

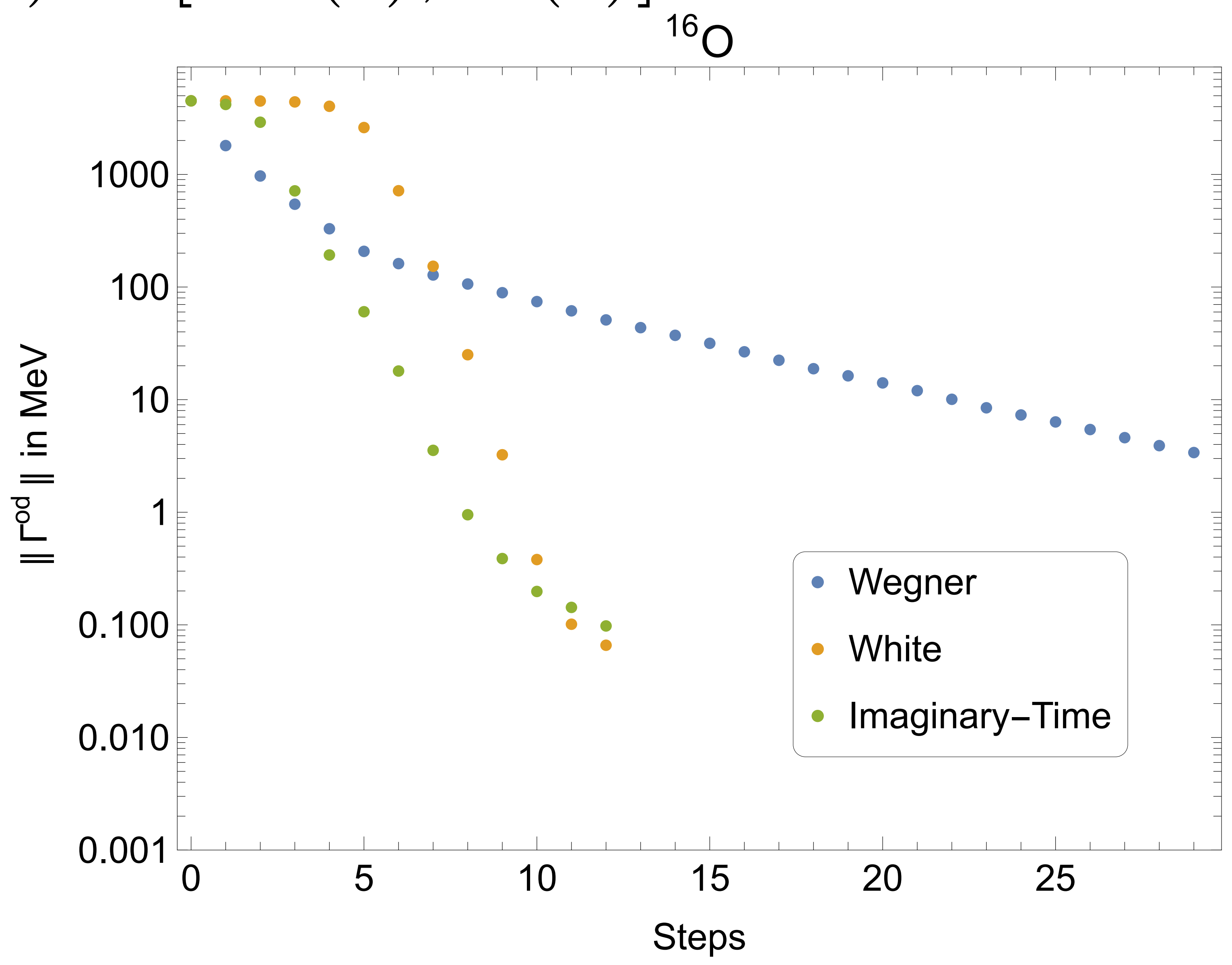
H. Hergert: In-Medium Similarity Renormalization Group for Closed and Open-Shell Nuclei, Phys. Scripta 92, 023002 (2017)

# Generators

- Wegner generator leads to stiff flow equation $\eta_{\text{Wegner}}(s) = [H^{\mathrm{d}}(s), H(s)]$
- White and imaginary-time generator

$$\eta(s) = \sum_{\substack{v \in V \\ w \in W}} \langle v|H(s)|w\rangle \, \mathcal{F}\Big( \langle w|H(s)|w\rangle - \langle v|H(s)|v\rangle \Big) \, |v\rangle \langle w| - h.c. \,,$$

$$\mathcal{F}(\Delta) = \begin{cases} \frac{1}{\Delta} & \text{for the White generator} \\ \operatorname{sgn}(\Delta) & \text{for the imaginary-time generator.} \end{cases}$$




- White generator faster, but imaginary-time generator more stable