



Online Meeting

South Africa – China Joint Research Programme

2024 – 2025

Meeting ID: 344 165 046 611
Passcode: zzxb33
@ Microsoft Teams meeting

**Thanks Prof. Anwar
for this online meeting!**

Jan. 29, 2024

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01 Idea about the Joint Research

“Tensor-Network State-based Quantum System Simulations by AI-supported HPC framework”

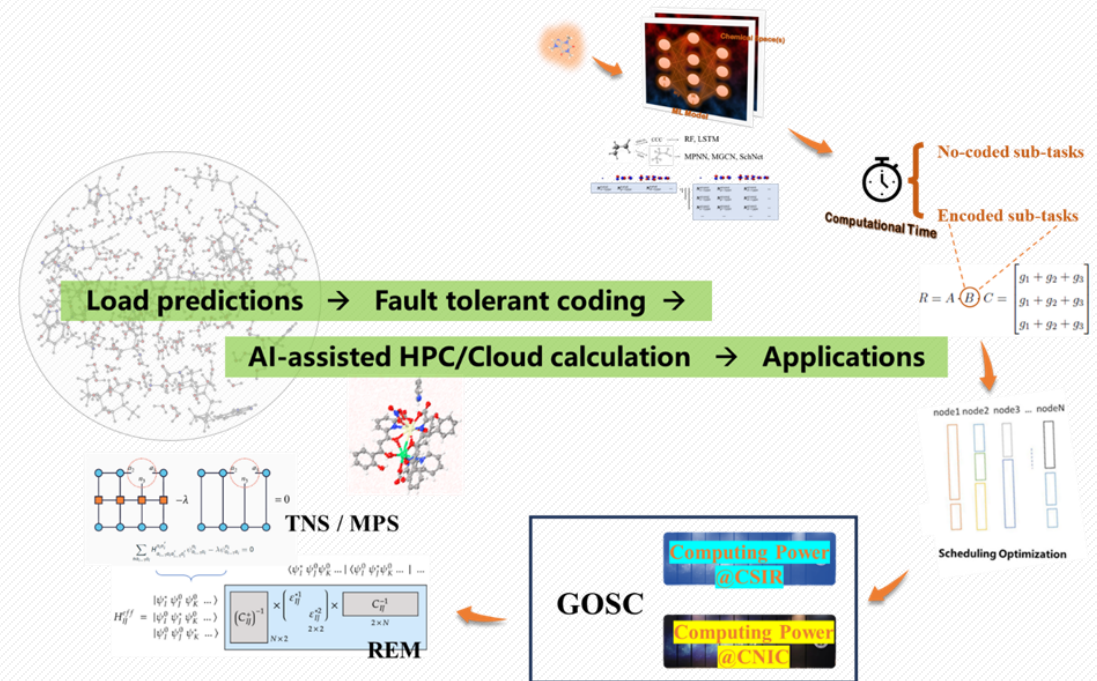
02 Related works @ CNIC

03 Planned tasks

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01 Idea about the Joint Research

“Tensor-Network State-based Quantum System Simulations by AI-supported HPC framework”



01 Idea about the Joint Research



中国科学院计算机网络信息中心
Computer Network Information Center,
Chinese Academy of Sciences

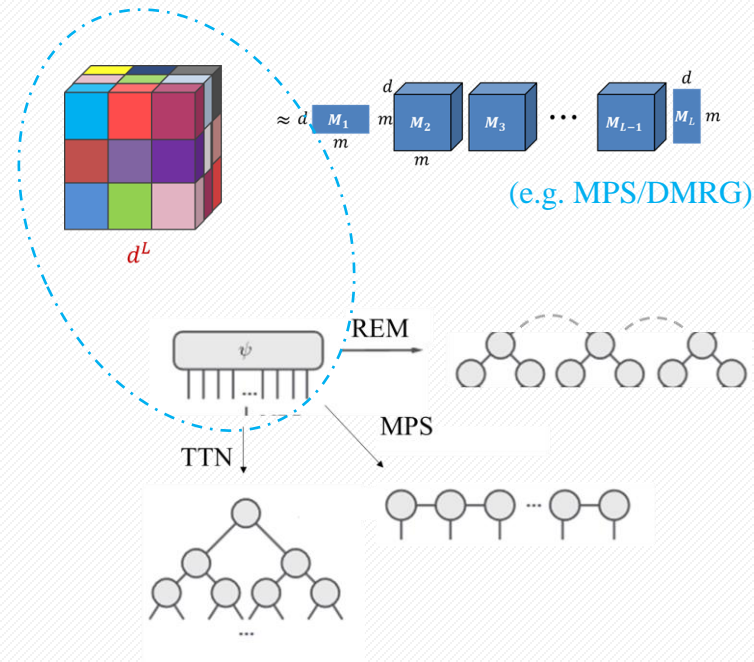
Tensor-Network State-based Quantum System Simulations by AI-supported HPC framework

(Physics)

(Chemistry)

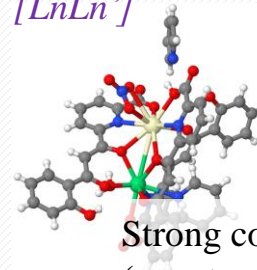
(Software/Algorithm)

(Hardware/Infrastructure)



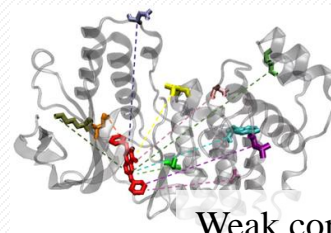
Quantum processor prototype molecule

Heterodimetallic
 $[LnLn']$

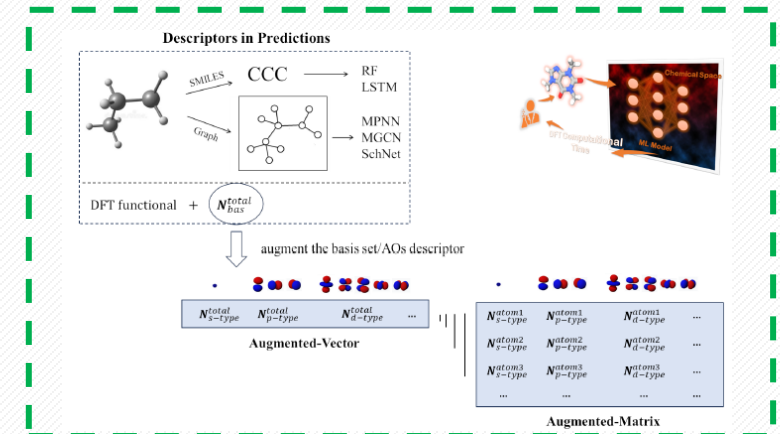


Strong correlated
(quantum super-position)

Protein-Ligand



Weak correlated
(Simple system)



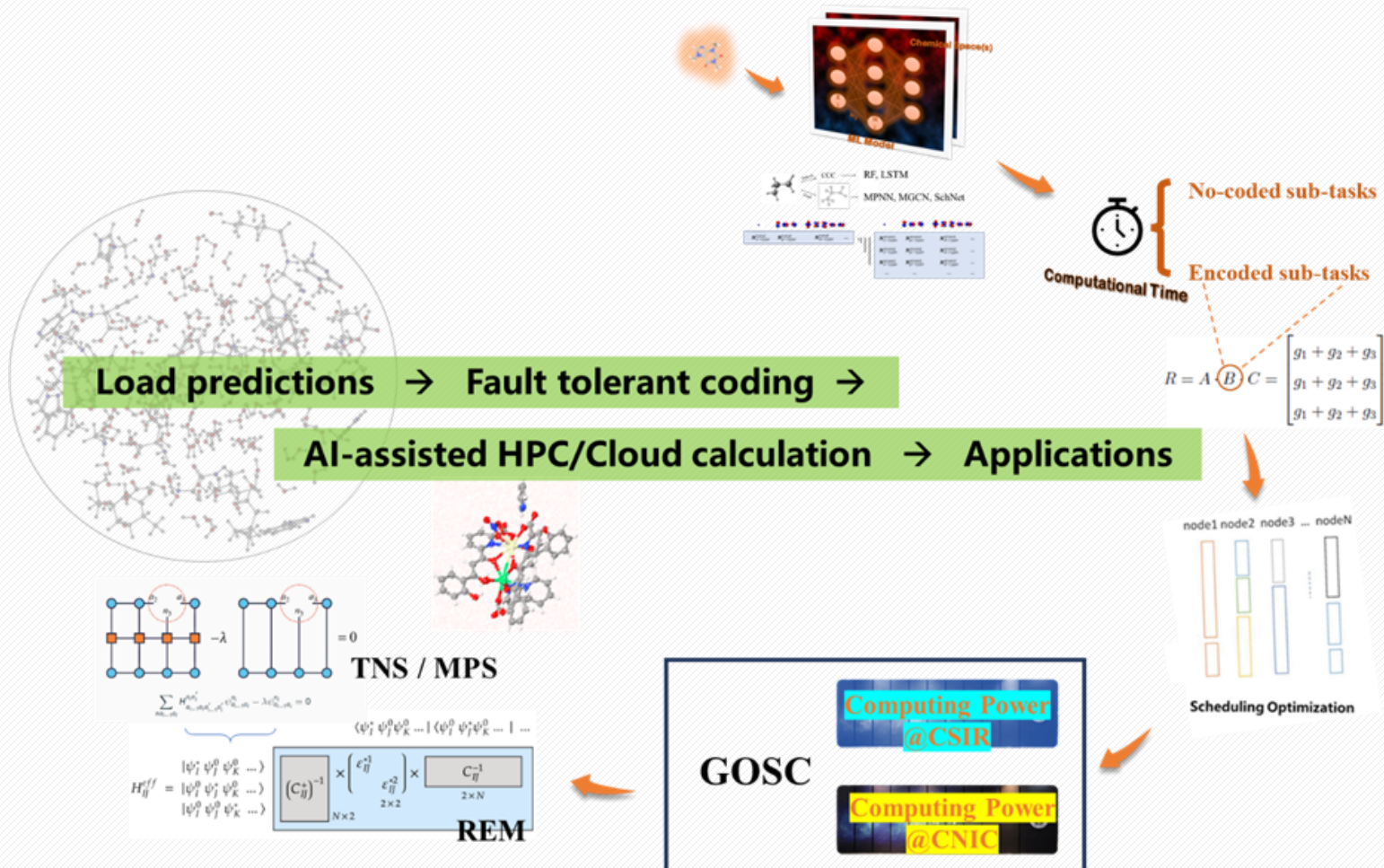
GOSC

Computing Power
@CSIR

Computing Power
@CNIC

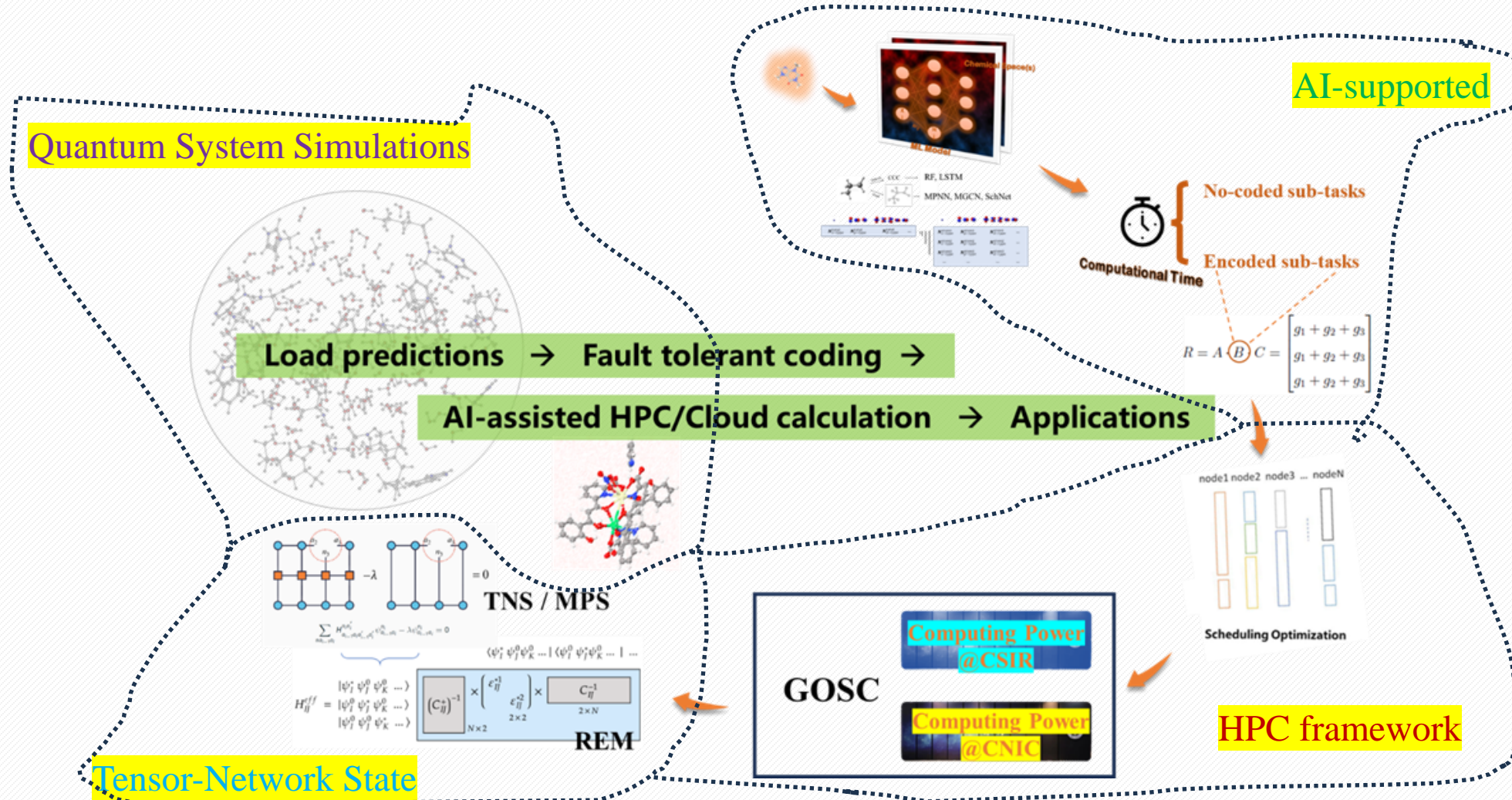
01 Idea about the Joint Research

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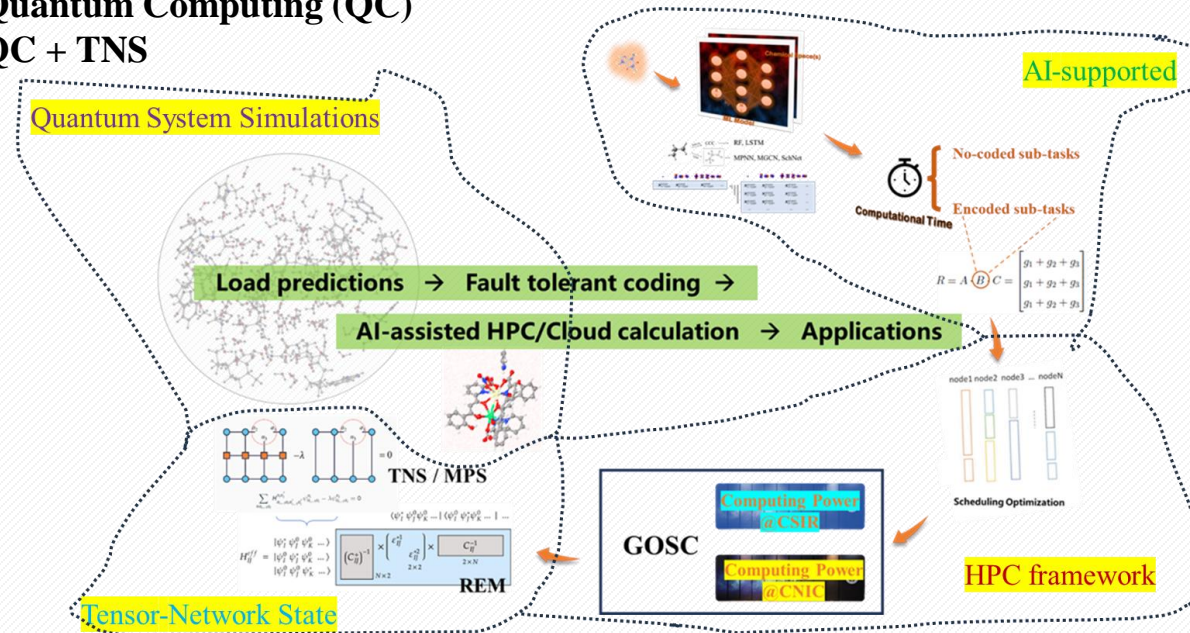


01 Idea about the Joint Research

Tensor-Network State-based Quantum System Simulations by AI-supported HPC framework

CSIR emphasis:

Quantum Computing (QC)
QC + TNS



1. C. & C. both contribute the GOSC (AOSP & CSTCloud), and have the purpose of description of quantum chemical / physics problems using the GOSC-related resources

2. CNIC places some emphasis on tensor-network approach, AI-assisted/coded (cross-domain) HPC calculations

3. CSIR places some emphasis on quantum computing, and combination with tensor-network approach

CNIC emphasis:

TNS @ AI/coded HPC

C. & C. both contribute the GOSC

01 Idea about the Joint Research

Tensor-Network State-based Quantum System Simulations by AI-supported HPC framework

@Anwar @Coral @Kelvin:

CSIR emphasis:

Quantum Computing (QC)

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@Yingjin @Qian @Baohua

CNIC emphasis:

TNS @ AI/coded HPC

@Lili @Happy @Mervyn @Nyameko @Yuepeng

C. & C. both contribute the GOSC

CONTENTS

02 **Related works @ CNIC**

02 Related works @ CNIC

@Lili @Happy @Mervyn @Nyameko @Yuepeng
C. & C. both contribute the GOSC

@Yingjin @Qian @Baohua

CNIC emphasis:

TNS @ AI/coded HPC

Governance for global research resources	Applications	Global Research collaboration Open science applications, open access, open collaboration, UN SDGs, Big Science Programs, research collaborations.
	Soft.&T.	Social community for open research resources SAAS level services and tools for different research resources, such as open access to journals
	Data	Global open data fabric
	Comp.	Cloud federation Computing, storage and analysis.
	Network	Global research & education network CSTNET, CERNET, ESnet, Internet2, GÉANT, AARNet, RedCLARA, SANReN
		Alliance for security, trusts and sustainability

“Network-for-Science”

- **Global R&E network**
- scalable, end-to-end, software-based for global networking connectivity.
- **Cloud Federation**
- flexible, dynamic, enhanced environment based on existing computing infrastructures and services following “Cloud” paradigms.
- **Global Open Data Fabric**
- optimal solutions to data management and capacity building for big data analytics.
- **Cloud Services for Science Community**
- multi-site cloud-based facilities and resources to support research across applications, services, and systems for the science community.
- **Global Research Collaboration**

02 Related works @ CNIC

@Lili @Happy @Mervyn @Nyameko @Yuepeng
C. & C. both contribute the GOSC

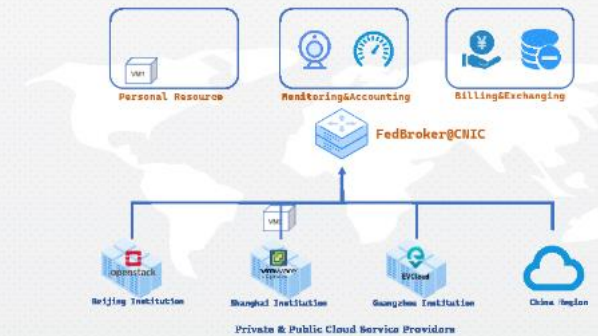
@Yingjin @Qian @Baohua
CNIC emphasis:
TNS @ AI/coded HPC

“Network-for-Science”

GOSC FedBroker@CNIC: The Gateway towards to the Open Science Cloud Infrastructures of CHINA.

GOSC FedBroker@CNIC is a FedBroker instance deployed by China Science and Technology Cloud. As a resource pool, GOSC FedBroker@CNIC integrates heterogeneous computing, storage and data resources of Chinese scientific research institutions in Beijing, Shanghai, Guangzhou, etc.; as a resource gateway, global users can uniformly access China's open scientific resources through FedBroker@CNIC.

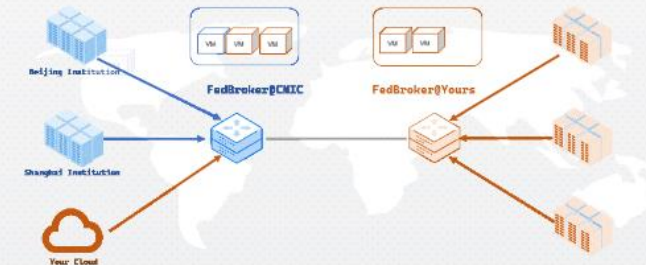
[READ MORE](#)



Invitation to Collaborate: Build The Resource Sharing Network With GOSC FedBroker@CNIC

In order to realize the GOSC initiative, we invite global scientific research institutions to build a global open science resource sharing network with GOSC FedBroker@CNIC. You can act as a service provider of GOSC FedBroker@CNIC, and GOSC FedBroker@CNIC provides services to scientific researchers on behalf of your resources; you can also deploy a GOSC FedBroker to exchange and share resources with us.

[READ MORE](#)



02 Related works @ CNIC

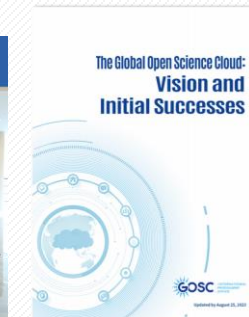
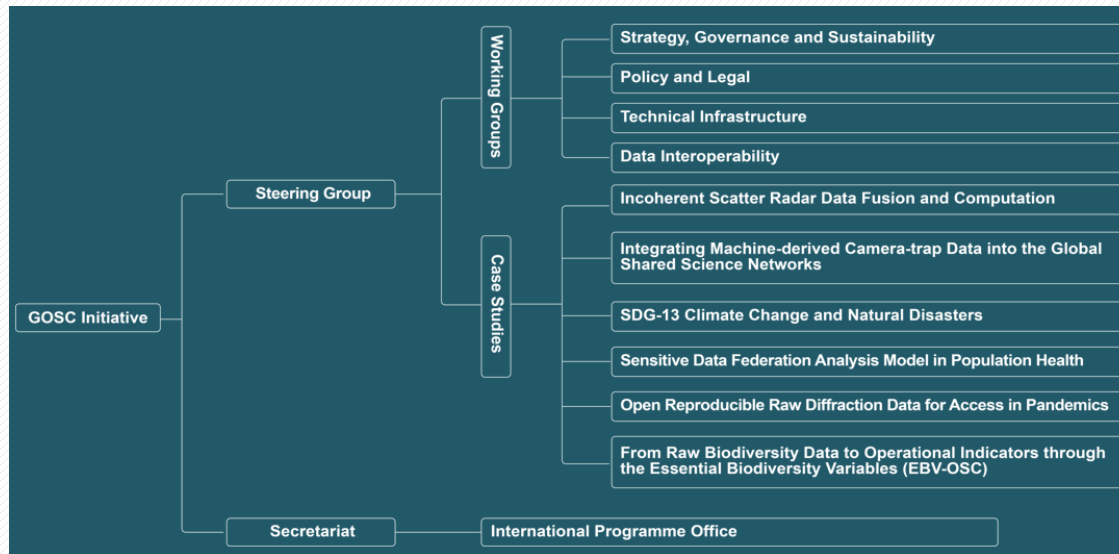


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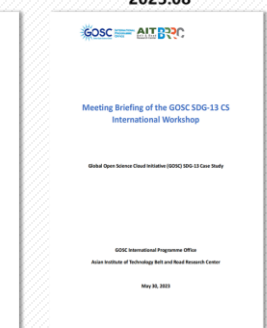
“Network-for-Science”



GOSC White Paper 2023.08



GOSC Report 2022 2023.08



GOSC SDG-13 Meeting Briefing 2023.05

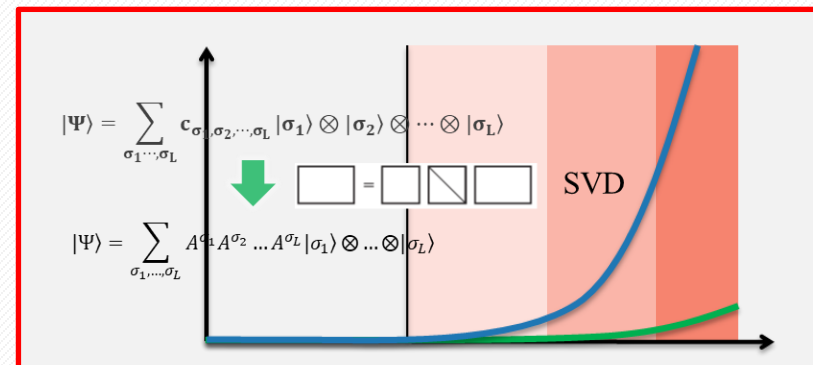
CAPACITY BUILDING & COMMUNITY OUTREACH

02 Related works @ CNIC "HPC/AI-for-Science"

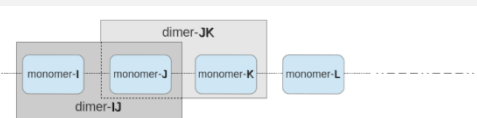
@Lili @Happy @Mervyn @Nyameko @Yuepeng
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Different correlated (quantum superposition) systems



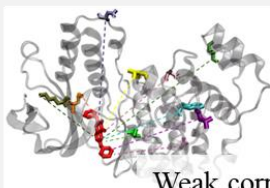
Divide and Conquer



N monomers, m states for each monomers

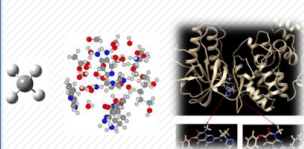
$$H^{eff} = \sum_{I=1}^N H^{eff}_I + \sum_{I>J} H^{eff}_{I,J} + \sum_{I>J>K} H^{eff}_{I,J,K} + \dots$$

Protein-Ligand



Weak correlated (Simple system)

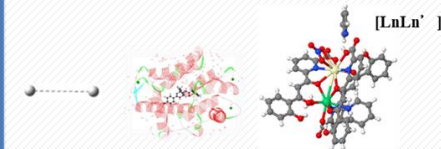
Weak correlated systems (Most equilibrium molecules)



- SR
- (HF, DFT, MP2, ...)
- Relatively low-scaling

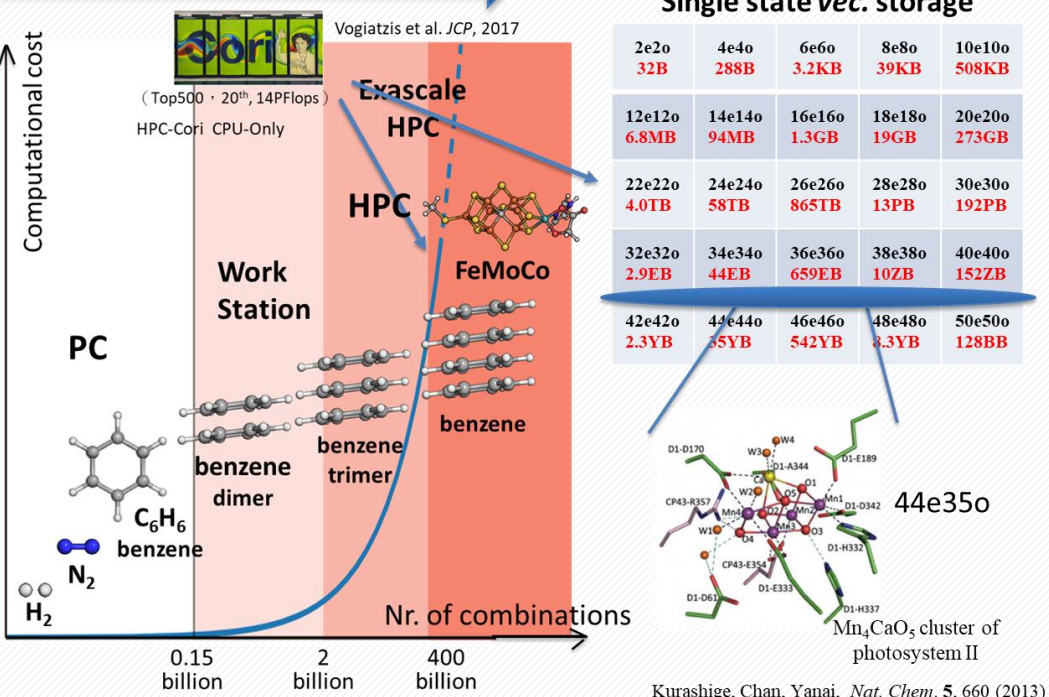
$$|\Psi\rangle = |\Psi_0\rangle$$

Strong correlated systems (Dissociated / excited / transition metal / ...)



- MC / MR
- (CASSCF, CASPT2, ...)
- Relatively high-scaling

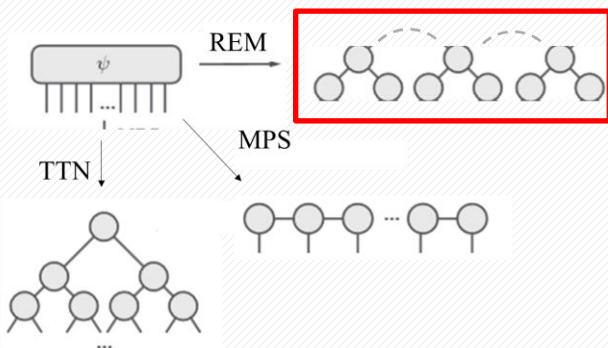
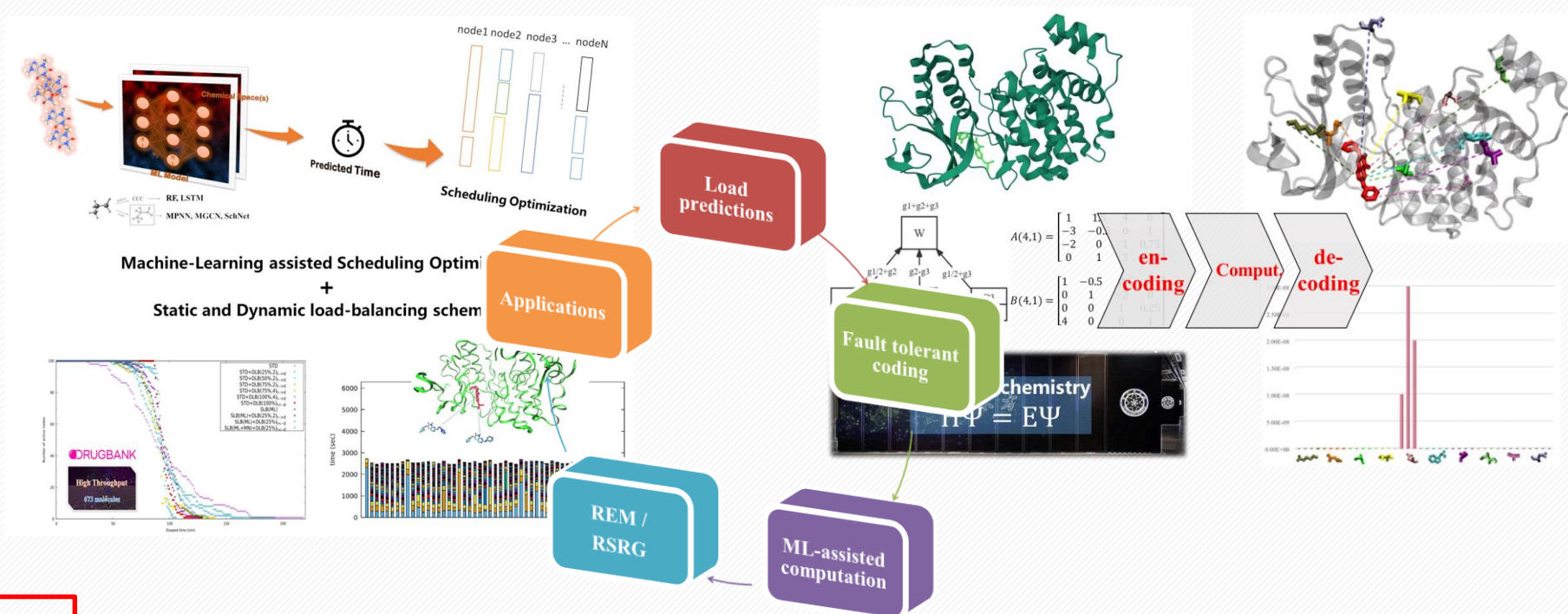
$$|\Psi\rangle = c_0|\Psi_0\rangle + c_1|\Psi_1\rangle + \dots + c_n|\Psi_n\rangle$$



02 Related works @ CNIC “HPC/AI-for-Science”

@Lili @Happy @Mervyn @Nyameko @Yuepeng
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$$H_{IJ}^{eff} = \begin{matrix} |\psi_i^* \psi_j^0 \psi_k^0 \dots\rangle \\ |\psi_i^0 \psi_j^* \psi_k^0 \dots\rangle \\ |\psi_i^0 \psi_j^0 \psi_k^* \dots\rangle \end{matrix} \langle \psi_i^* \psi_j^0 \psi_k^0 \dots | \langle \psi_i^0 \psi_j^* \psi_k^0 \dots | \dots$$

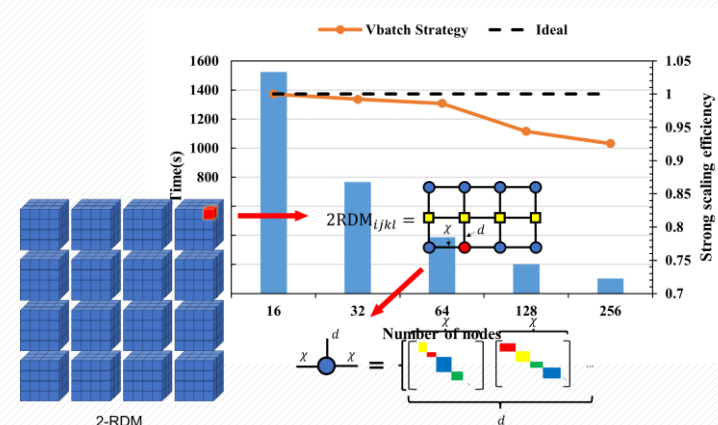
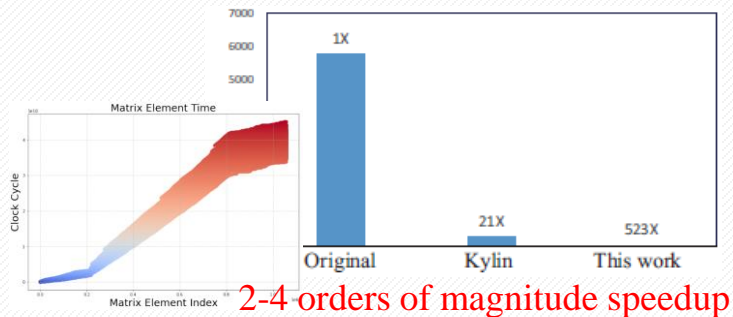
$$\begin{matrix} (C_{IJ}^+)^{-1} & \times & \begin{pmatrix} \varepsilon_{IJ}^{*1} \\ & \varepsilon_{IJ}^{*2} \end{pmatrix} & \times & C_{IJ}^{-1} \\ N \times 2 & & 2 \times 2 & & 2 \times N \end{matrix}$$

ACS Omega, **6**, 2001 (2021)
Comput. Sci. (CN), **49**, 36 (2022)
J. Comput. Chem. **44**, 1174 (2023)
Acta Chim. Sin. (CN), 10.6023/A23110496 (2024)
J. Comput. Chem. in revision (ArXiv:2401.09484)

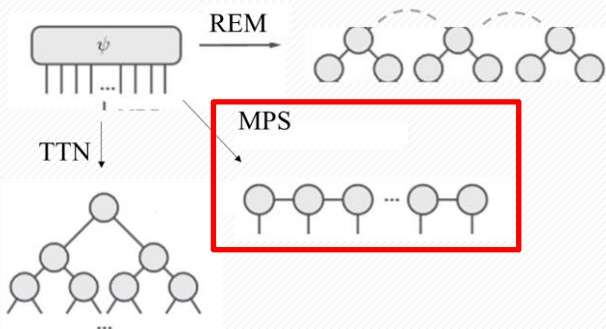
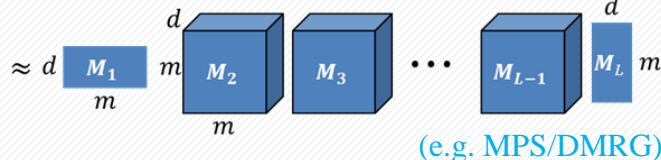
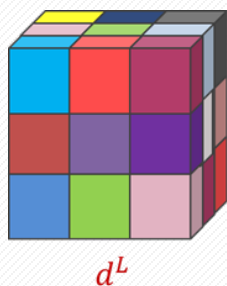
02 Related works @ CNIC “HPC/AI-for-Science”

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Strong scaling (GPU_vbatch) > 92%



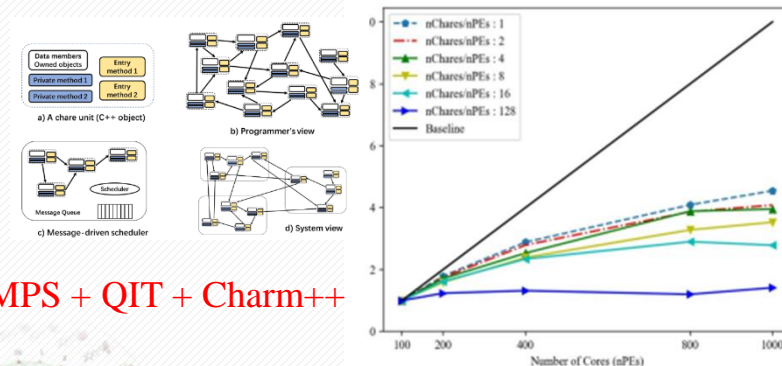
(two-site)
 $|\Psi_{\text{MPS}}\rangle = \sum_{\sigma_1, \dots, \sigma_L} A_{1\sigma_1}^{\sigma_1} \dots A_{l-1, \sigma_{l-1}}^{\sigma_{l-1}} M_{\sigma_{l-1}, \sigma_l}^{\sigma_{l-1}, \sigma_l} B_{\sigma_l, \sigma_{l+1}}^{\sigma_l, \sigma_{l+1}} \dots B_{L, \sigma_L}^{\sigma_L}$

Conf.-Orb. Coupling
(2nd order SCF)

Gradients
(Coupled-Perturbed)

Geom. Opt.
CI point Opt.

Method developments



J. Comput. Chem. **41**, 2707 (2020)
J. Comput. Chem. **44**, 1316 (2023)
J. Chem. Theory Comput. **13**, 2533 (2017)
J. Chem. Theory Comput. **15**, 6724 (2019)
Phys. Chem. Chem. Phys. **22**, 4957 (2020)
 HPCC – 2023, accepted
 ICS 2024, submitted

CONTENTS

03

Planned tasks

Tensor-Network State-based Quantum System Simulations by AI-supported HPC framework

(Physics)

(Chemistry)

(Software/Algorithm)

(Hardware/Infrastructure)

@Anwar @Coral @Kelvin:

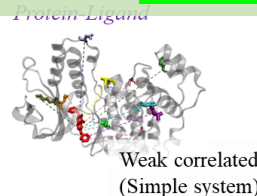
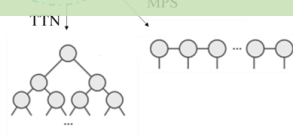
CSIR emphasis:

Quantum Computing (QC)

QC + TNS

Cooperation (basic) : everyone does his/her own field of expertise, meanwhile, try to

- docking the latest developments in **computational approach/software** by TNS
- docking the latest developments in **“Network-for -Science”** by GOSC



@Yingjin @Qian @Baohua

CNIC emphasis:

TNS @ AI/coded HPC

GOSC

Computing Power
@CSIR

Computing Power
@CNIC

@Lili @Happy @Mervyn @Nyameko @Yuepeng
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(Physics)

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Quantum Computing (QC)
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QC for quantum chemistry (?)

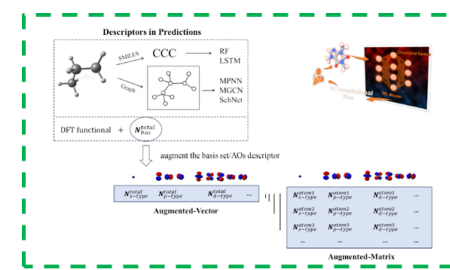
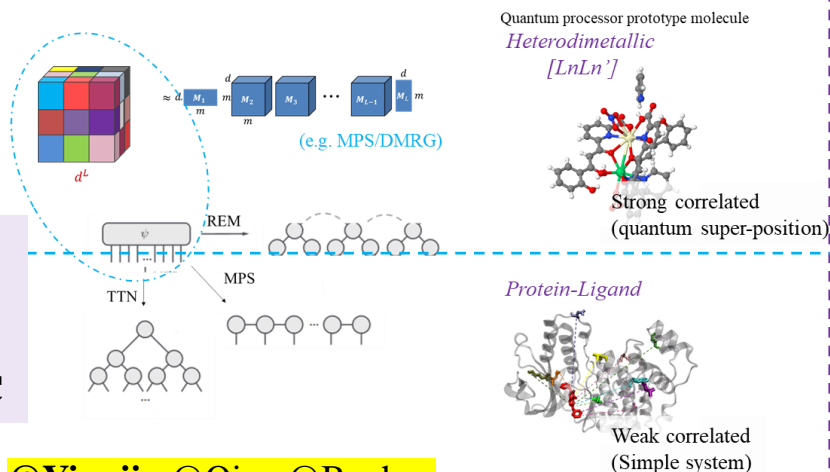
- *ab initio* Hamiltonian
- Strong- and weak-correlated
- Interface to GOSC/TNS

Multi-Scale TNS

- Hardware adaptive
- Coded calculation
- Interface to GOSC/QC

@Yingjin @Qian @Baohua

CNIC emphasis:
TNS @ AI/coded HPC



GOSC

Computing Power
@CSIR

Computing Power
@CNIC

GOSC & Testbed

- Cross-domain
- Fault-tolerant
- ENV support for QC/TNS

@Lili @Happy @Mervyn @Nyameko @Yuepeng
C. & C. both contribute the GOSC

Thanks for your attention!

