Shapes and Symmetries in Nuclei: from Experiment to Theory (SSNET'18)
Nov. 5, 2018, CNRS, Gif-sur-Yvette, France

Recent progress of nuclear dynamics studies with TDDFT

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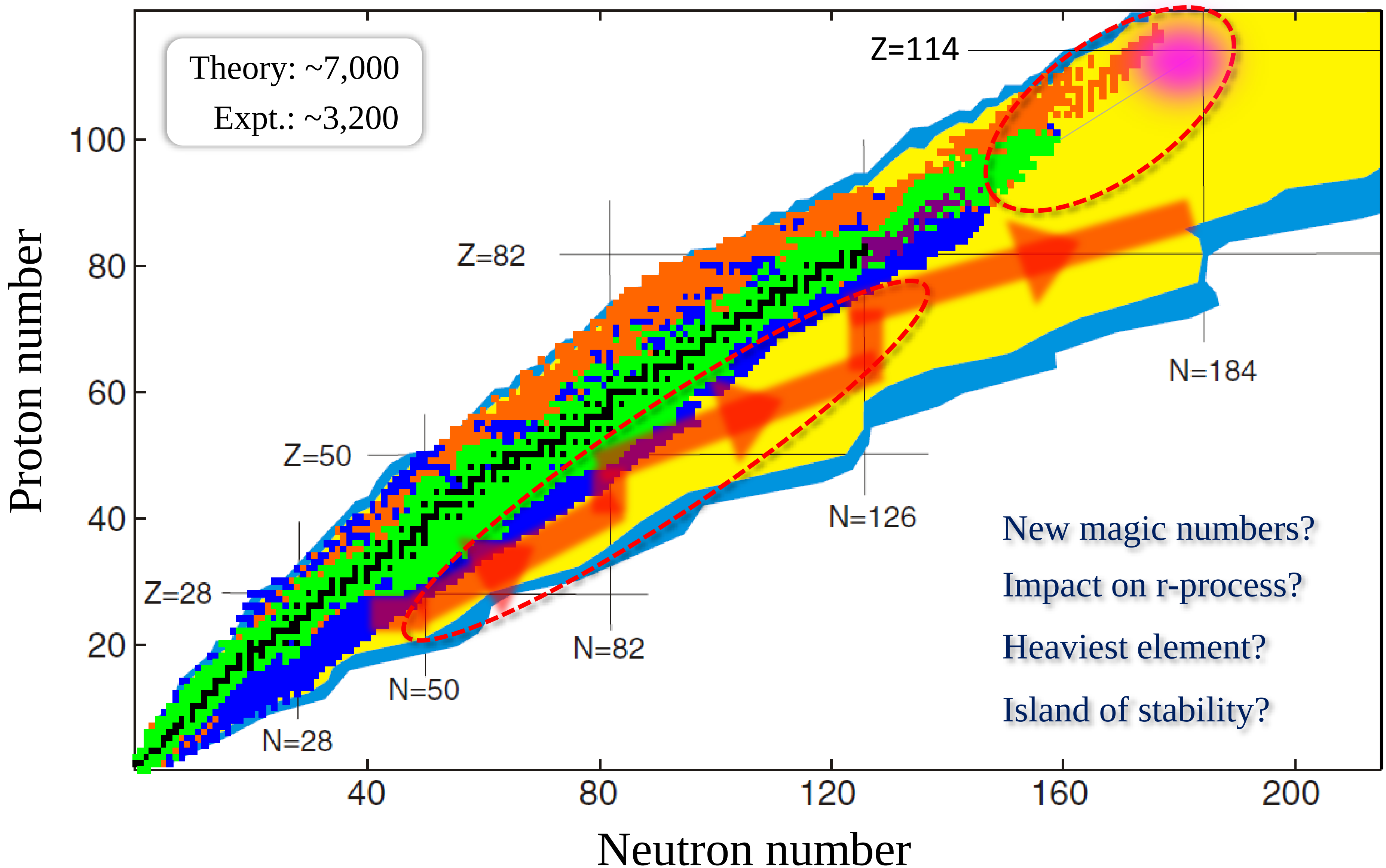
Center for Interdisciplinary Research
Institute for Research Promotion, Niigata University, Japan

Progress #1

Development of "TDHF+GEMINI" for unstable nucleus production

How can we create yet-unknown neutron-rich nuclei?



New magic numbers?

Impact on r-process?

Heaviest element?

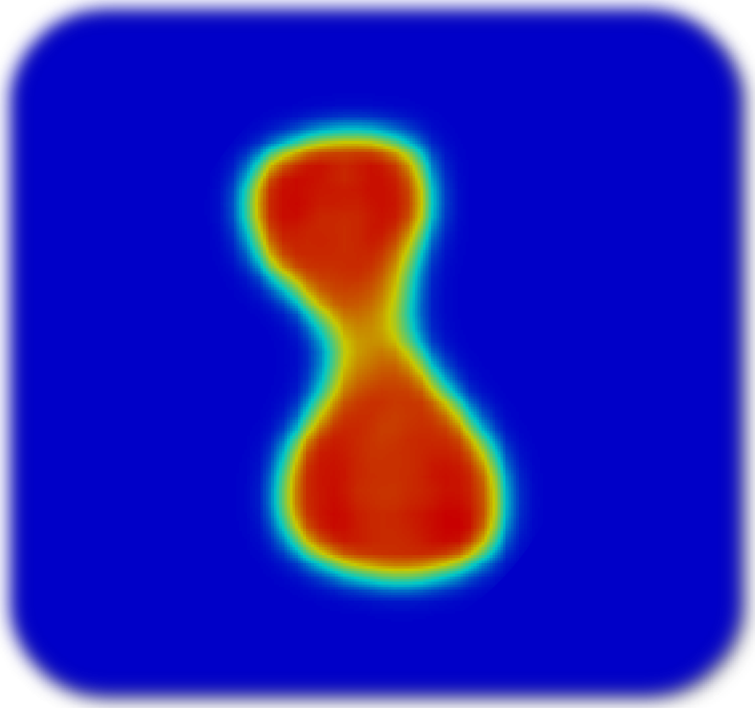
Island of stability?

M. Thoennessen, Rep. Prog. Phys. **76**, 056301 (2013)

How to compute production cross sections?

We have developed: **TDDFT + PNP + GEMINI**

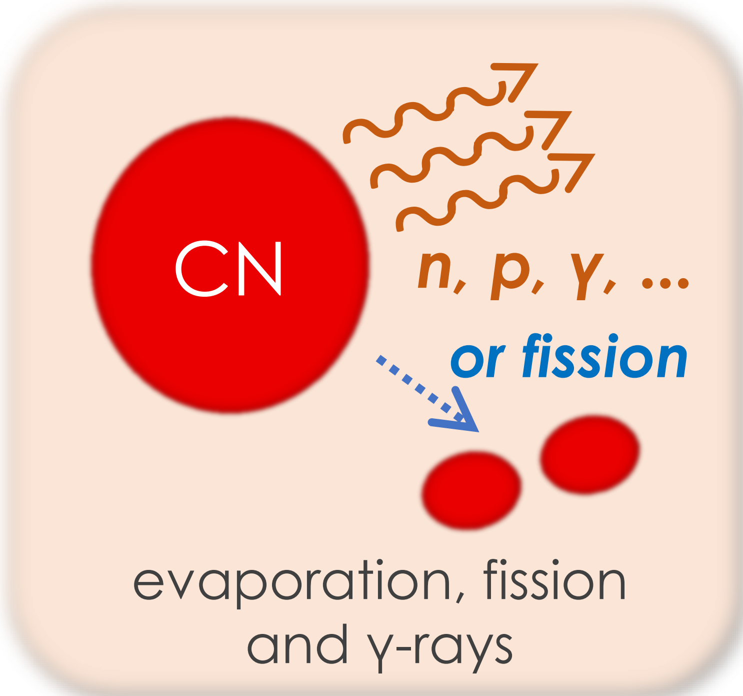
TDDFT



Reaction dynamics
(10^{-21}-10^{-20} sec)

+

GEMINI++



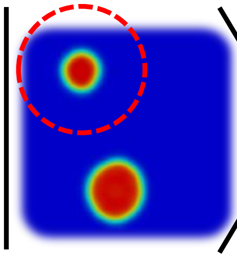
De-excitation
(10^{-18}-10^{-16} sec)

We have developed: **TDDFT + PNP + GEMINI**

✓ Particle number projection (PNP)

C. Simenel, PRL105(2010)192701

$$\left|\Phi_{N,Z}(b)\right\rangle = \hat{P}_N \hat{P}_Z \left|\Phi(b)\right\rangle = \hat{P}_N \hat{P}_Z \left| \quad \right\rangle$$



PNP operator:

$$\hat{P}_n = \frac{1}{2\pi}\int_0^{2\pi} e^{i(n-\hat{N}_V)\theta} d\theta$$

- Transfer probabilities and cross sections

KS and K. Yabana, PRC**88**(2013)014614

$$P_{N,Z}(b) = \left\langle \Phi_{N,Z}(b) \middle| \Phi_{N,Z}(b) \right\rangle = P_N(b) P_Z(b)$$

$$\sigma_{N,Z} = 2\pi \int b\, P_{N,Z}(b) db$$

- Expectation values

KS and K. Yabana, PRC**90**(2014)064614

$$\mathcal{O}_{N,Z}(b) = \frac{\left\langle \Phi_{N,Z}(b) \middle| \hat{\mathcal{O}}_V \middle| \Phi_{N,Z}(b) \right\rangle}{\left\langle \Phi_{N,Z}(b) \middle| \Phi_{N,Z}(b) \right\rangle}$$

$$J_{N,Z}(b),\ E^*_{N,Z}(b)$$

Inputs for a statistical model

- Secondary deexcitation processes

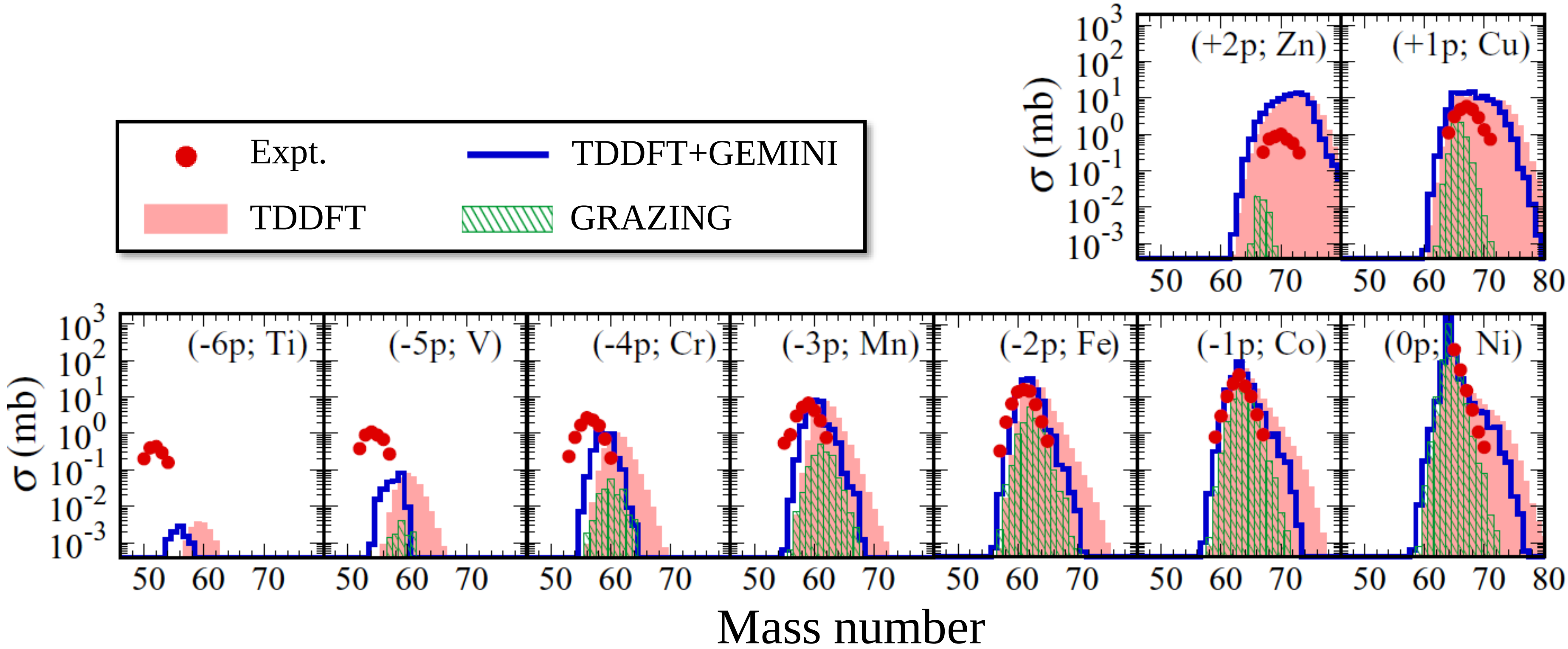
KS, PRC**96**(2017)014615

Evaporation/Fission/Gamma by GEMINI++ [R.J. Charity, PRC**82**(2010)014610]

TDHF vs. Expt. - $^{64}Ni+^{238}U$ ($E_{c.m.}$=307 MeV)

KS and K. Yabana, PRC**88**(2013)014614; KS, PRC**96**(2017)014615

Production cross section for projectile-like fragments



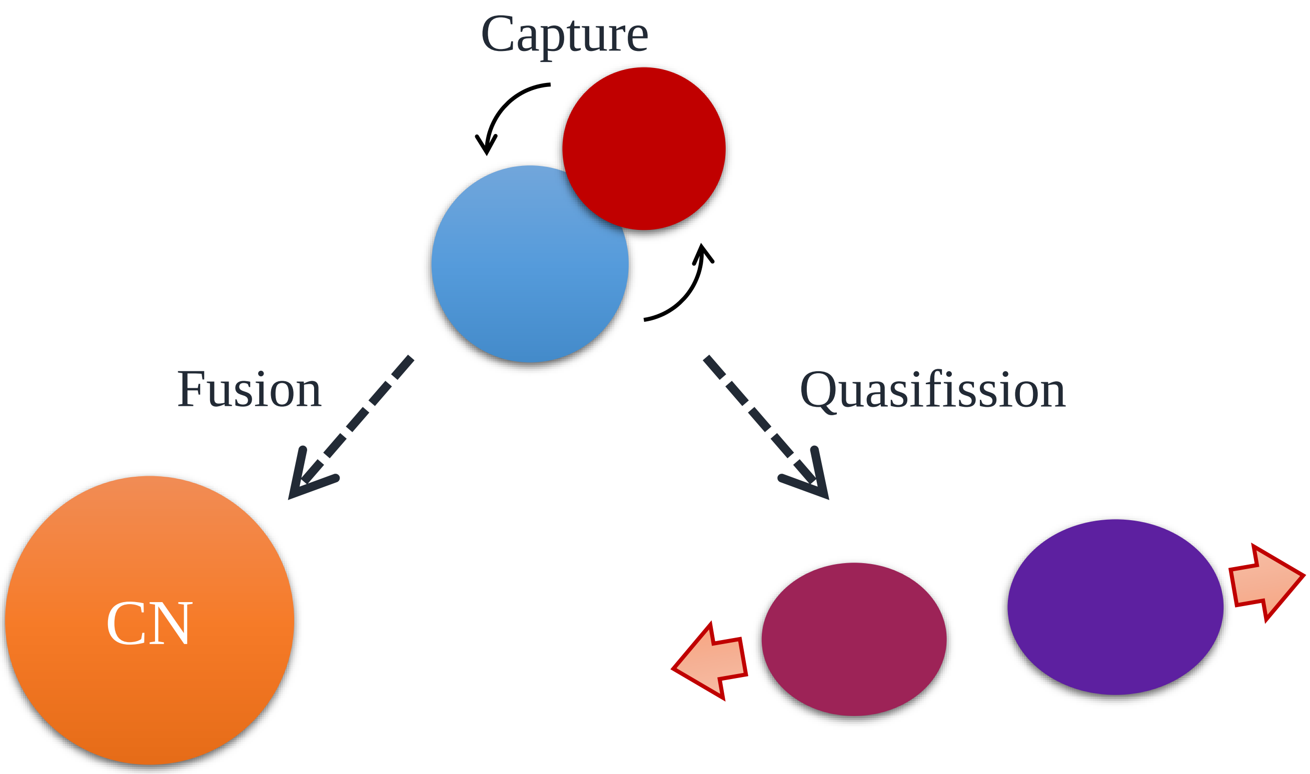
Expt.: L. Corradi et al., PRC**59**(1999)261

Progress #2

<u>Study of Quasifission dynamics</u>

Quasifission process

A fast (~10^{-21}-10^{-20} sec) fission process before compound nucleus formation (fusion)



$$\sigma_{\rm ER} \sim W_{\rm surv} * \sigma_{\rm cap} * P_{\rm CN}$$

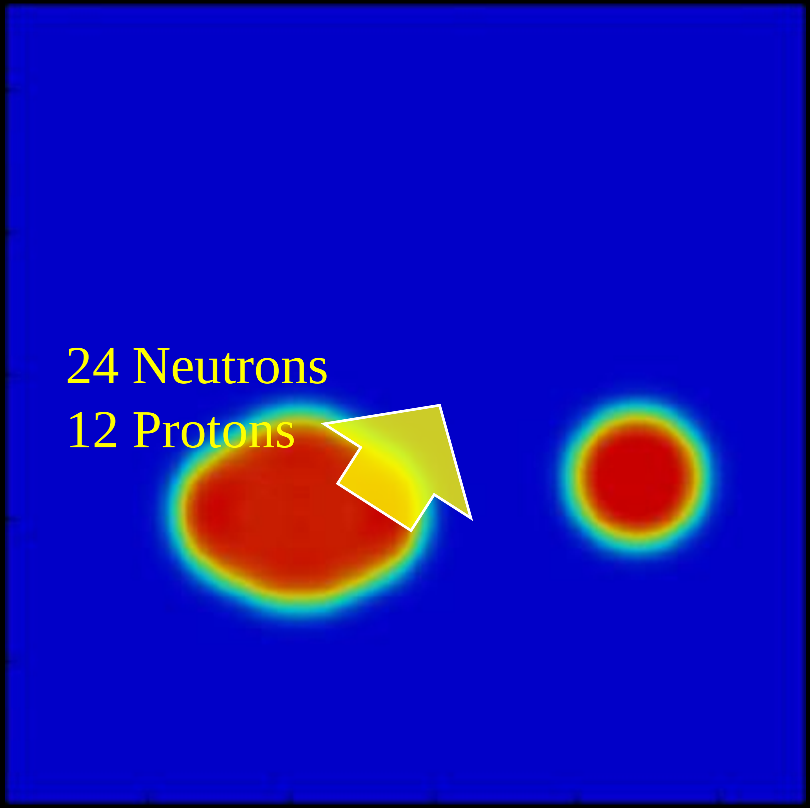
$^{64}Ni+^{238}U$ at E_{lab}=390 MeV

KS and K. Yabana, PRC**93**(2016)054616

Quasifission dynamics in TDHF

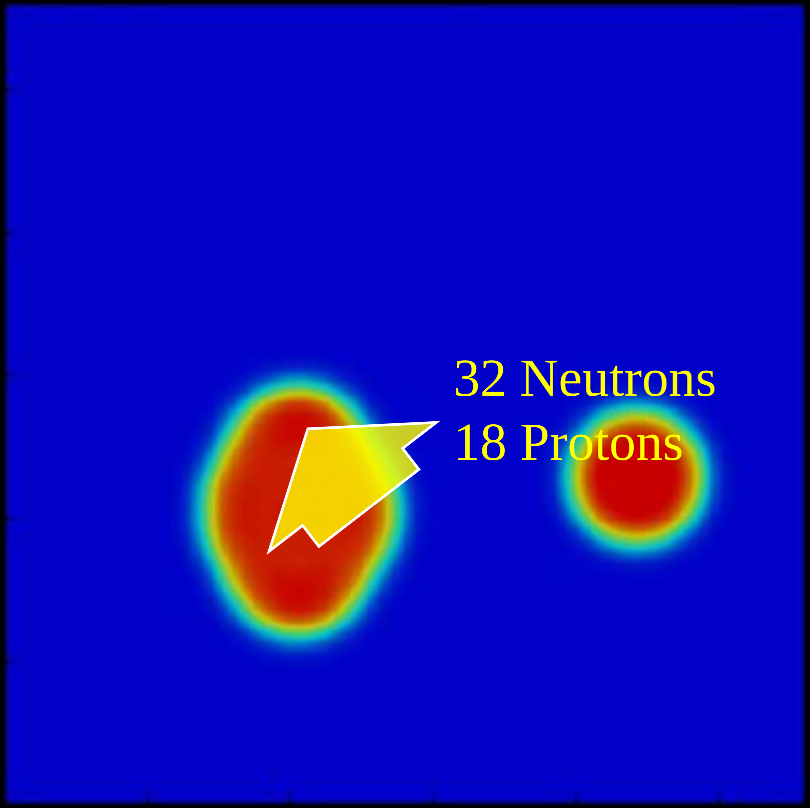
Tip collision

Shell effects of ^{208}Pb



Side collision

More mass-symmetric

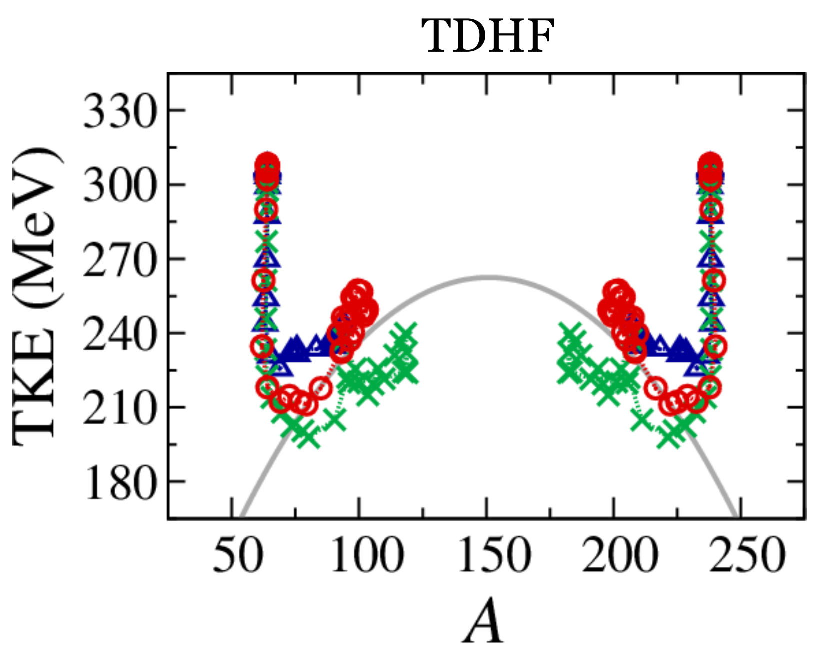


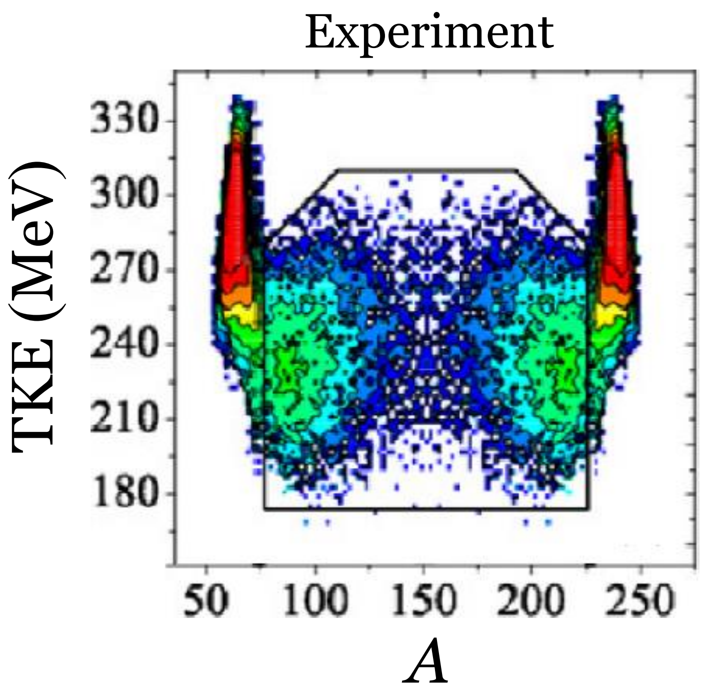
$^{64}Ni+^{238}U$ at E_{lab}=390 MeV

KS and K. Yabana, PRC**93**(2016)054616

TDHF provides quantitative description of quasifission dynamics

TKE-*A* distribution: Comparison with experimental data





Expt.: E.M. Kozulin *et al.*, PLB**686**(2010)227

Progress #3

<u>Quantitative description of the mass width in DIC</u>

This work is based on our recent PRL paper:

PHYSICAL REVIEW LETTERS **120,** 022501 (2018)

Exploring Zeptosecond Quantum Equilibration Dynamics: From Deep-Inelastic to Fusion-Fission Outcomes in $^{58}Ni + ^{60}Ni$ Reactions

E. Williams,[1,*] K. Sekizawa,[2] D. J. Hinde,[1] C. Simenel,[1] M. Dasgupta,[1] I. P. Carter,[1] K. J. Cook,[1] D. Y. Jeung,[1] S. D. McNeil,[1] C. S. Palshetkar,[1,†] D. C. Rafferty,[1] K. Ramachandran,[1,‡] and A. Wakhle[1]
[1]*Department of Nuclear Physics, Research School of Physical Sciences and Engineering, The Australian National University, Canberra, ACT 2601, Australia*
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(Received 16 August 2017; revised manuscript received 27 October 2017; published 10 January 2018)

performed in collaboration with *Australian National University* (ANU)

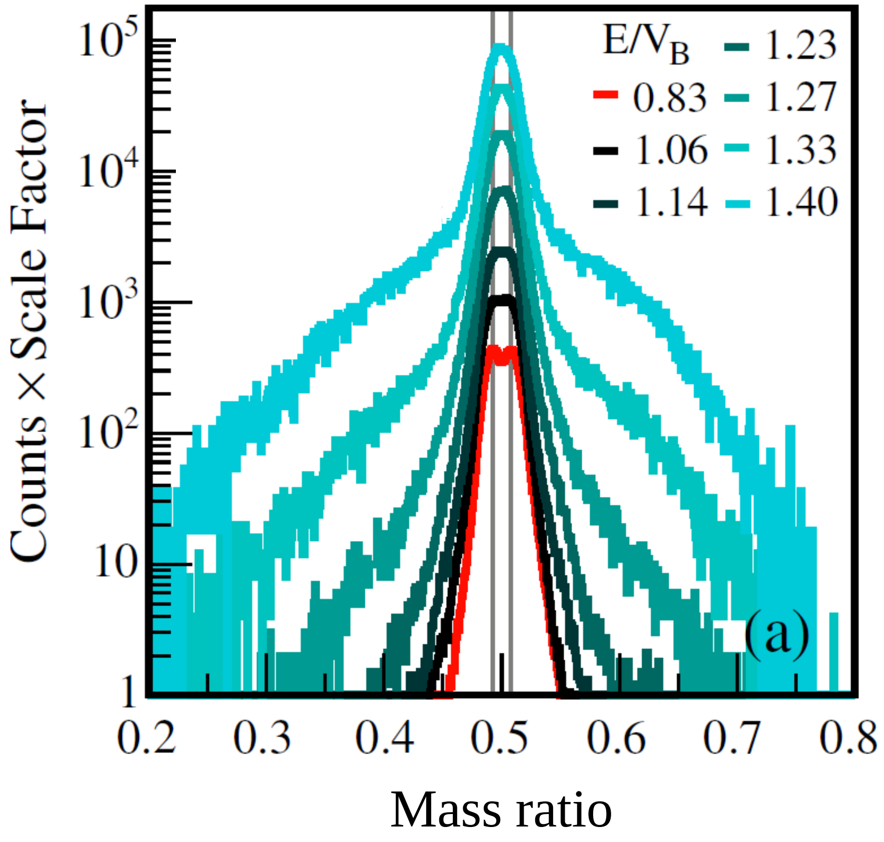

E. Williams


D.J. Hinde


M. Dasgupta


C. Simenel

Mass distributions of ^{58}Ni+^{60}Ni at various energies



Mass ratio:

$$M_R = \frac{M_i}{M_1 + M_2}$$

Variational space can be controlled by "state" and "observable"

- The action-like quantity defined by Balian and Vénéroni

$$J = \mathrm{Tr}\left[\hat{A}(t_1)\hat{D}(t_1)\right] - \int_{t_0}^{t_1} \mathrm{Tr}\left[\hat{A}(t)\left(\frac{d\hat{D}(t)}{dt} + i\left[\hat{H}(t), \hat{D}(t)\right]\right)\right] dt$$

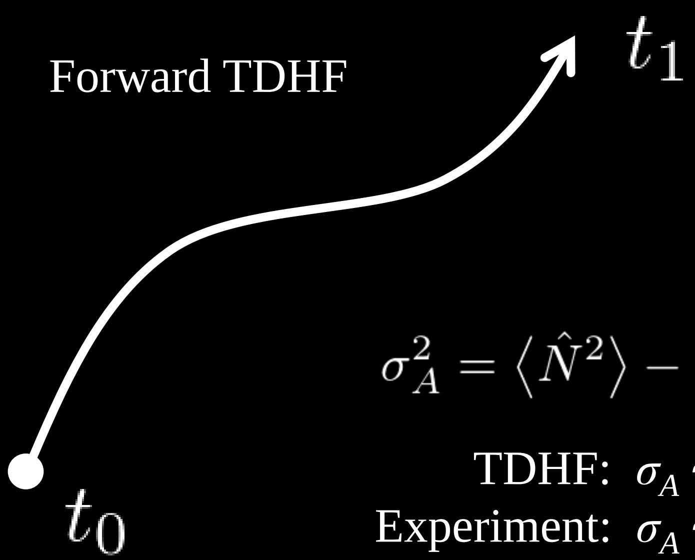
$\hat{D}(t)$: describes the state of the system

$\hat{A}(t)$: describes the evolution of the observable in the Heisenberg picture

R. Balian and M. Vénéroni, Phys. Rev. Lett. **47**, 1353 (1981); Ann. Phys. **216**, 351 (1992).
C. Simenel, Phys. Rev. Lett. **106**, 112501 (2011); Eur. Phys. J. A **48**, 152 (2012).

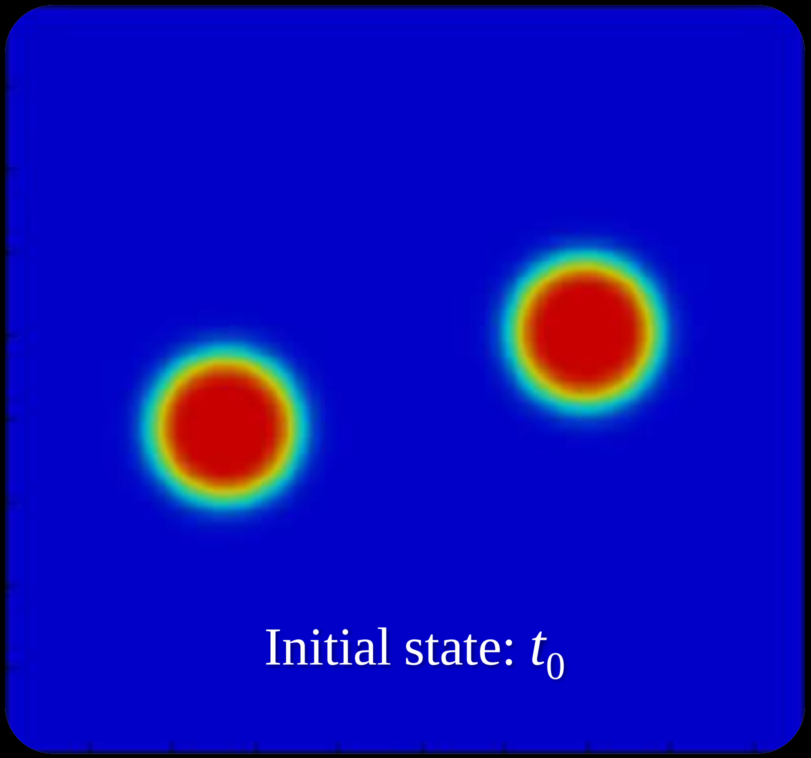
- **Unrestricted variation** (w.r.t. either *A* or *D*) → **TDSE**
- **Slater determinant** & one-body observable → **TDHF**
- **Slater determinant** & fluctuations of one-body observable → **TDRPA**

Numerical implementation of BV prescription for the mass width



$$\sigma_A^2 = \langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2$$

TDHF: $\sigma_A \sim 1.5$
Experiment: $\sigma_A \sim 7.1$



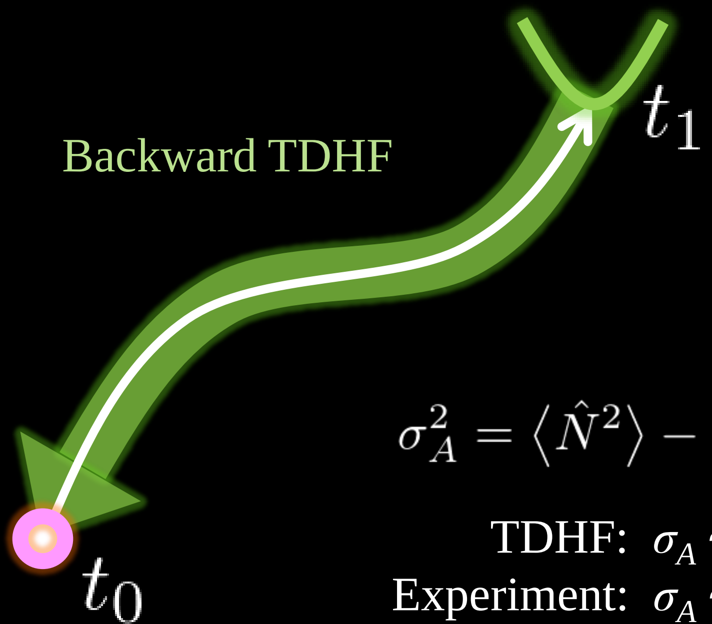
R. Balian and M. Vénéroni, Phys. Rev. Lett. **47**, 1353 (1981); Ann. Phys. **216**, 351 (1992).
C. Simenel, Phys. Rev. Lett. **106**, 112502 (2011); Eur. Phys. J. A **48**, 152 (2012).

Numerical implementation of BV prescription for the mass width

The Balian-Vénéroni prescription:

$$\sigma_X^2(t_1) = \lim_{\varepsilon \to 0} \frac{\mathrm{Tr}\{[\rho(t_0) - \rho_X(t_0, \varepsilon)]^2\}}{2\varepsilon^2}$$

$$\rho_X(t_1, \varepsilon) = e^{i\varepsilon \hat{X}} \rho(t_1) e^{-i\varepsilon \hat{X}}$$



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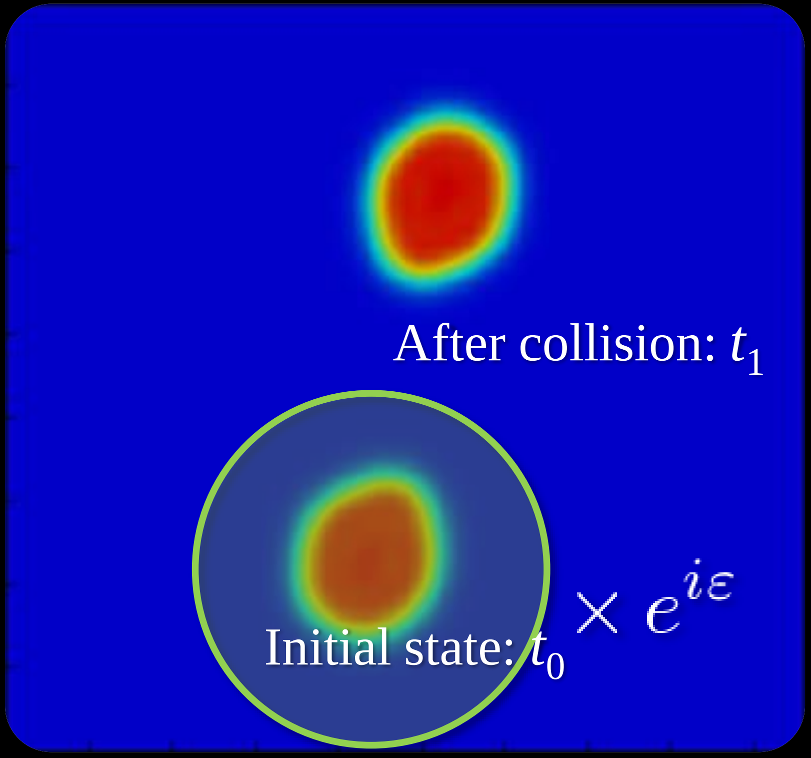


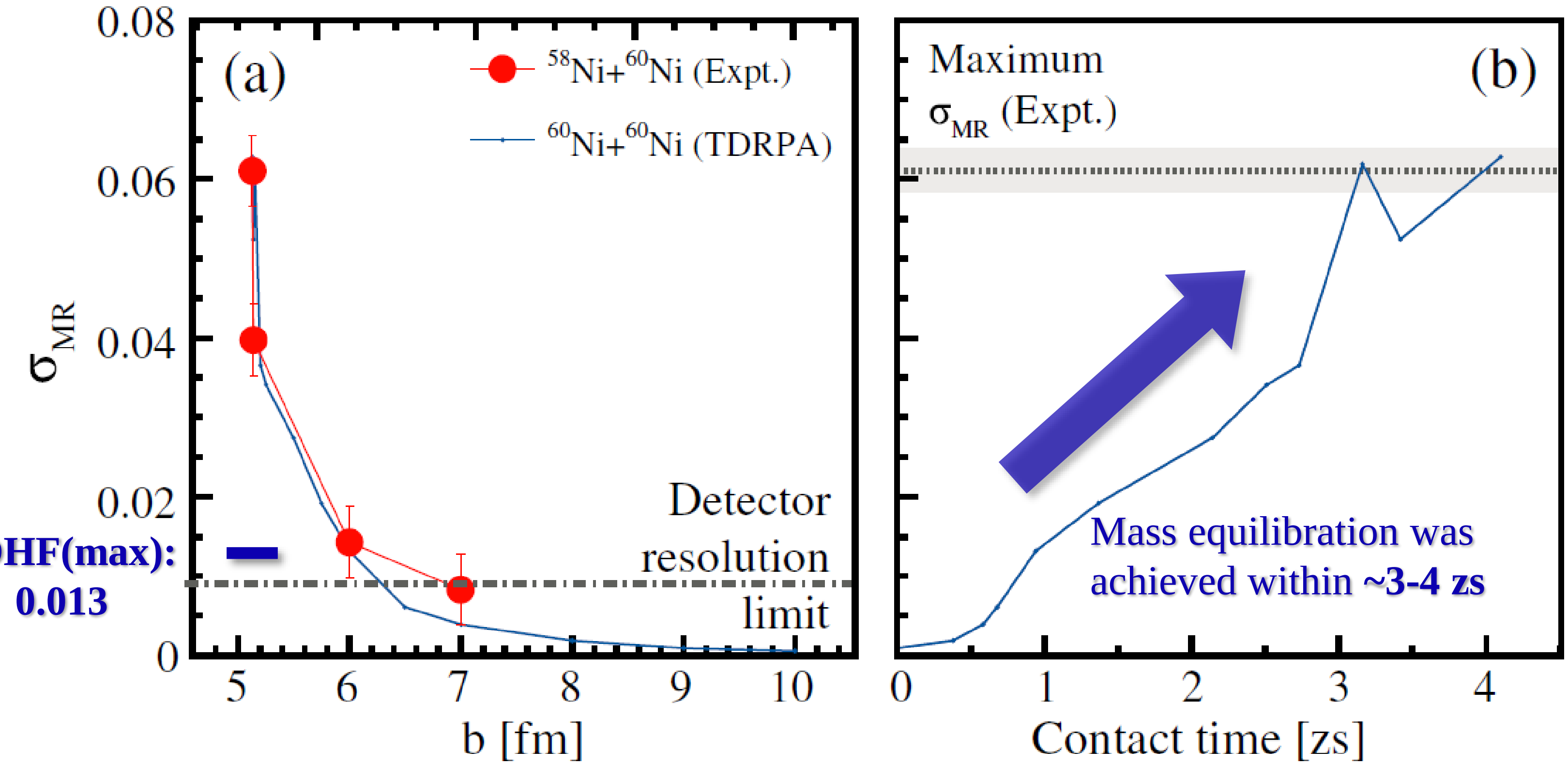
R. Balian and M. Vénéroni, Phys. Rev. Lett. **47**, 1353 (1981); Ann. Phys. **216**, 351 (1992).
C. Simenel, Phys. Rev. Lett. **106**, 112502 (2011); Eur. Phys. J. A **48**, 152 (2012).

$^{58,60}Ni+^{60}Ni$ at $E/V_B=1.4$

E. Williams, K. Sekizawa, D. Hinde *et al.*, Phys. Rev. Lett. **120**, 022501 (2018)

TDRPA quantitatively reproduced the experimental data

Width of the mass ratio distribution, σ_{MR}: Expt. vs Theory



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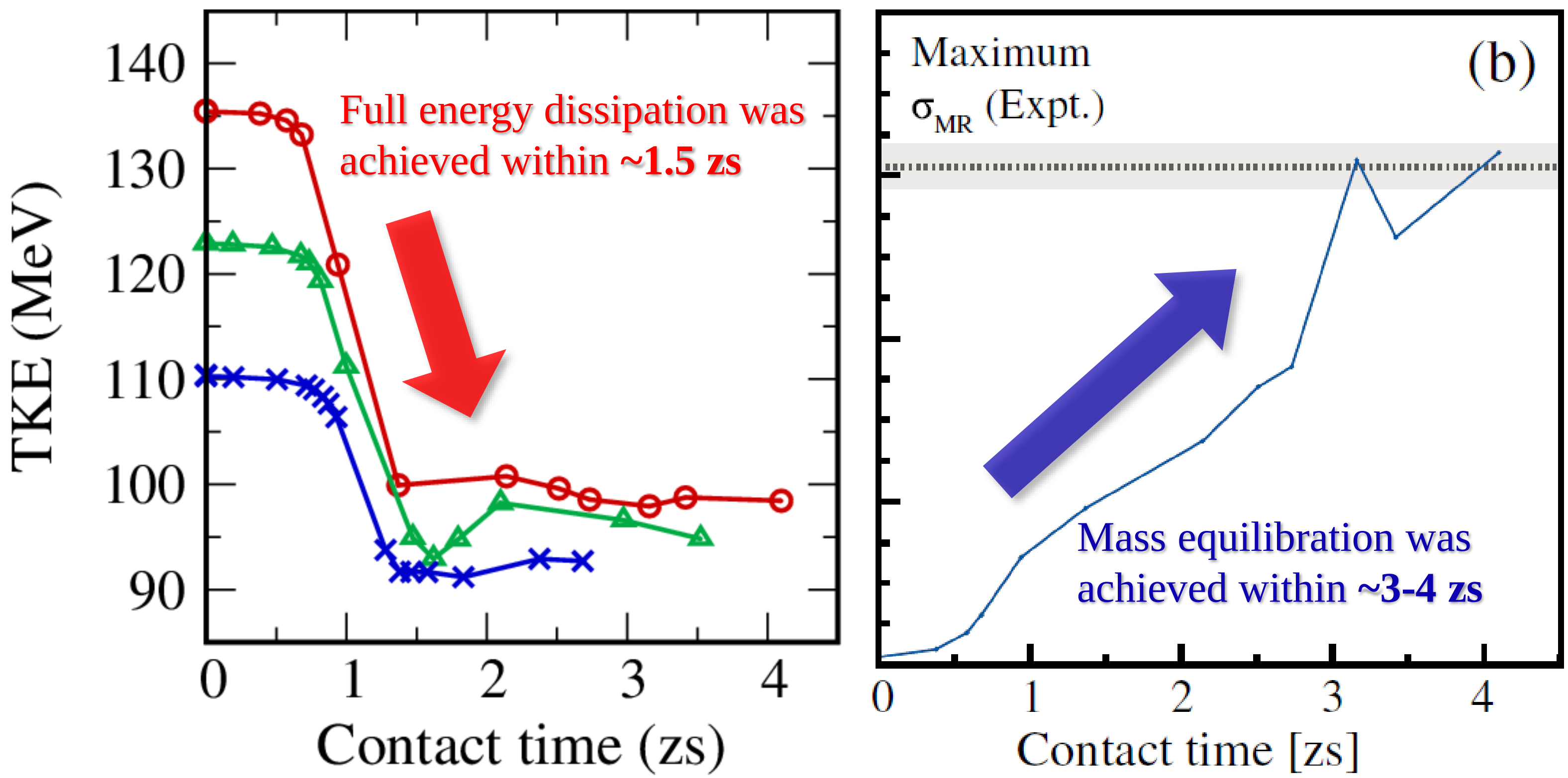

What's more?

Inclusion of pairing - TDSLDA

TDSLDA: TDDFT with local treatment of pairing

Kohn-Sham scheme is extended for non-interacting quasiparticles

- TDSLDA equations (formally equivalent to TDHFB or TD-BdG equations)

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{k,\uparrow}(\boldsymbol{r},t) \\ u_{k,\downarrow}(\boldsymbol{r},t) \\ v_{k,\uparrow}(\boldsymbol{r},t) \\ v_{k,\downarrow}(\boldsymbol{r},t) \end{pmatrix} = \begin{pmatrix} h_{\uparrow\uparrow}(\boldsymbol{r},t) & h_{\uparrow\downarrow}(\boldsymbol{r},t) & 0 & \Delta(\boldsymbol{r},t) \\ h_{\downarrow\uparrow}(\boldsymbol{r},t) & h_{\downarrow\downarrow}(\boldsymbol{r},t) & -\Delta(\boldsymbol{r},t) & 0 \\ 0 & -\Delta^*(\boldsymbol{r},t) & -h^*_{\uparrow\uparrow}(\boldsymbol{r},t) & -h^*_{\uparrow\downarrow}(\boldsymbol{r},t) \\ \Delta^*(\boldsymbol{r},t) & 0 & -h^*_{\downarrow\uparrow}(\boldsymbol{r},t) & -h^*_{\downarrow\downarrow}(\boldsymbol{r},t) \end{pmatrix}\begin{pmatrix} u_{k,\uparrow}(\boldsymbol{r},t) \\ u_{k,\downarrow}(\boldsymbol{r},t) \\ v_{k,\uparrow}(\boldsymbol{r},t) \\ v_{k,\downarrow}(\boldsymbol{r},t) \end{pmatrix}$$

$h_\sigma = \dfrac{\delta E}{\delta n_\sigma}$: s.p. Hamiltonian

$\Delta = -\dfrac{\delta E}{\delta \nu^*}$: pairing field

$n_\sigma(\boldsymbol{r},t) = \sum_{E_k<E_c} |v_{k,\sigma}(\boldsymbol{r},t)|^2$: number density

$\nu(\boldsymbol{r},t) = \sum_{E_k<E_c} u_{k,\uparrow}(\boldsymbol{r},t) v^*_{k,\downarrow}(\boldsymbol{r},t)$: anomalous density

$\boldsymbol{j}_\sigma(\boldsymbol{r},t) = \hbar \sum_{E_k<E_c} \mathrm{Im}[v^*_{k,\sigma}(\boldsymbol{r},t)\boldsymbol{\nabla} v_{k,\sigma}(\boldsymbol{r},t)]$: current

A large number (10^4-10^6) of 3D coupled non-linear PDEs have to be solved!!

# of qp orbitals ~ # of grid points

TDSLDA (Time-Dependent Superfluid Local Density Approximation)

TDSLDA: TDDFT with local treatment of pairing

Kohn-Sham scheme is extended for non-interacting quasiparticles

➢ TDSLDA equations (formally equivalent to TDHFB or TD-BdG equations)

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{k,\uparrow}(\boldsymbol{r},t) \\ u_{k,\downarrow}(\boldsymbol{r},t) \\ v_{k,\uparrow}(\boldsymbol{r},t) \\ v_{k,\downarrow}(\boldsymbol{r},t) \end{pmatrix} = \begin{pmatrix} h_{\uparrow\uparrow}(\boldsymbol{r},t) & h_{\uparrow\downarrow}(\boldsymbol{r},t) & 0 & \Delta(\boldsymbol{r},t) \\ h_{\downarrow\uparrow}(\boldsymbol{r},t) & h_{\downarrow\downarrow}(\boldsymbol{r},t) & -\Delta(\boldsymbol{r},t) & 0 \\ 0 & -\Delta^*(\boldsymbol{r},t) & -h^*_{\uparrow\uparrow}(\boldsymbol{r},t) & -h^*_{\uparrow\downarrow}(\boldsymbol{r},t) \\ \Delta^*(\boldsymbol{r},t) & 0 & -h^*_{\downarrow\uparrow}(\boldsymbol{r},t) & -h^*_{\downarrow\downarrow}(\boldsymbol{r},t) \end{pmatrix}\begin{pmatrix} u_{k,\uparrow}(\boldsymbol{r},t) \\ u_{k,\downarrow}(\boldsymbol{r},t) \\ v_{k,\uparrow}(\boldsymbol{r},t) \\ v_{k,\downarrow}(\boldsymbol{r},t) \end{pmatrix}$$

Supercomputing!!

$$h_\sigma = \frac{\delta E}{\delta n_\sigma}$$: s.p. Hamiltonian

$$\Delta = -\frac{\delta E}{\delta \nu^*}$$: pairing field

$$n_\sigma(\boldsymbol{r},t) = \sum_{E_k<E_c} |v_{k,\sigma}(\boldsymbol{r},t)|^2$$: number density

$$\nu(\boldsymbol{r},t) = \sum_{E_k<E_c} u_{k,\uparrow}(\boldsymbol{r},t)v^*_{k,\downarrow}(\boldsymbol{r},t)$$: anomalous density

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A large number (10^4-10^6) of 3D coupled non-linear PDEs have to be solved!!

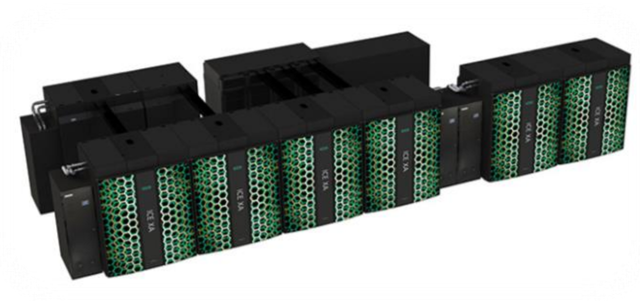
# of qp orbitals ~ # of grid points

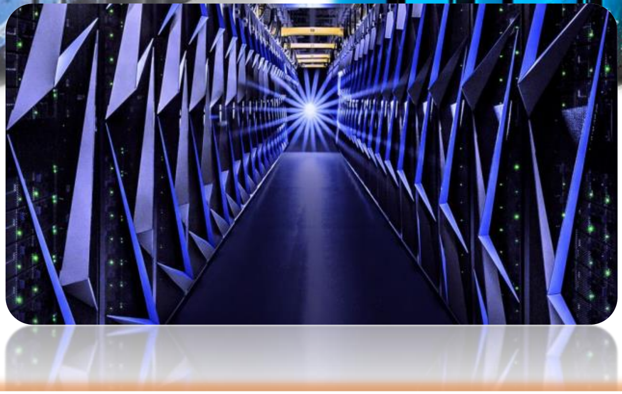
*The number indicates the rank according to the TOP500 list (June 2018)

Piz Daint, CSCS, Switzerland (No. 6)

TITAN, ORNL, USA (No. 7)

TSUBAME3.0, Japan (No. 19)

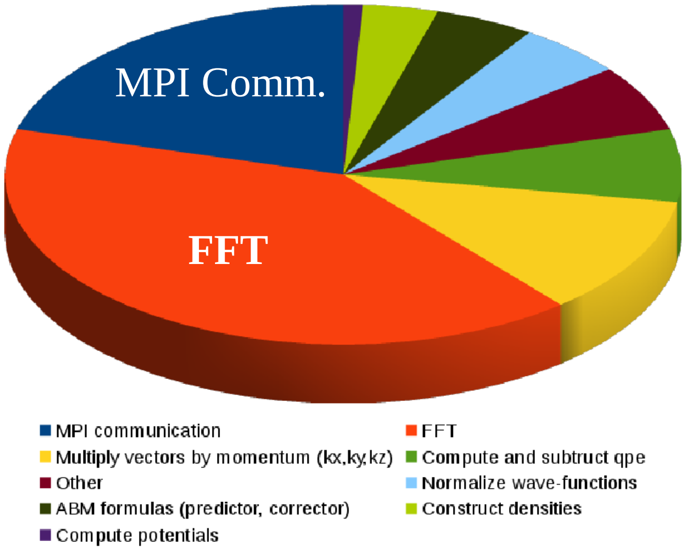




The fastest machine:
Summit, ORNL, USA
GPU, 188 PFlops/s

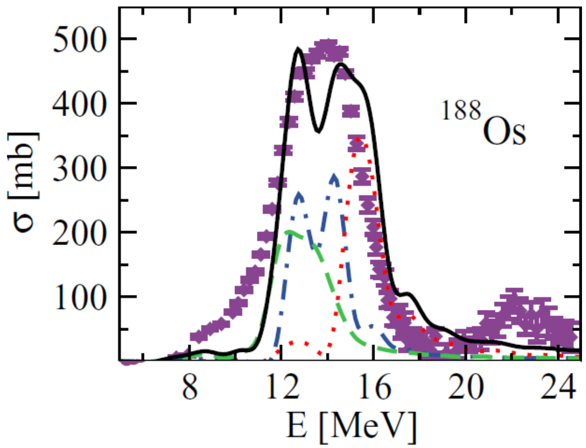
Present computing capabilities:

- ✓ Full 3D (w/o symmetry restrictions)
- ✓ Volume as large as 100^3 lattice points
- ✓ Evolution up to 10^6 time steps (as long as 10^{-19} sec)



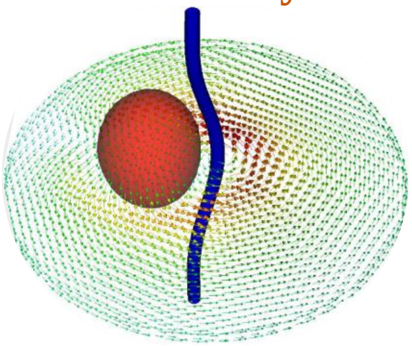
TDSLDA is a versatile tool!!

IVGDR



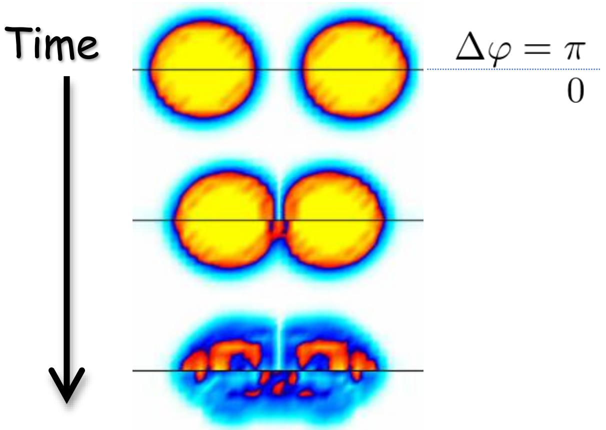
Phys. Rev. C **84**, 051309(R) (2011)
I. Stetcu, A. Bulgac, P. Magierski, and K.J. Roche

Vortex-nucleus dynamics



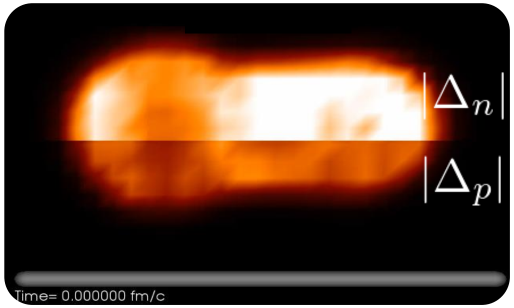
Phys. Rev. Lett. **117**, 232701 (2016)
G. Wlazłowski, K.S., P. Magierski, A. Bulgac, and M.M. Forbes

Low-energy heavy ion reactions



Phys. Rev. Lett. **119**, 042501 (2017)
P. Magierski, K.S., and G. Wlazłowski

Induced fission of ^{240}Pu



Phys. Rev. Lett. **116**, 122504 (2016)
A. Bulgac, P. Magierski, K.J. Roche, and I. Stetcu

Takeaway message

✓ One-body dissipation and fluctuation, together with the pairing, may be sufficient to describe various nuclear dynamics

Dynamic effects of pairing

TDHFB

Solitonic excitations, quantum vortices,
inner crust of neutron stars,
…

Main reaction outcomes

TDHF

Average number of nucleons,
TKE, scattering angles,
contact times, …

Fluctuations/correlations

TDRPA

Width of mass, charge distributions,
correlation between n/p transfers,
…

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