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Clean Numerical Simulation (CNS) and its applications

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1. Motivations

2. Clean Numerical Simulation (CNS)

3. Applications of the CNS

4. Concluding remarks and Discussions

1. Motivations

Characteristics of chaos

- **Sensitivity on initial condition (Poincare 1890s)**

a **small** change in one state of a deterministic nonlinear system can result in **large** differences in a later state

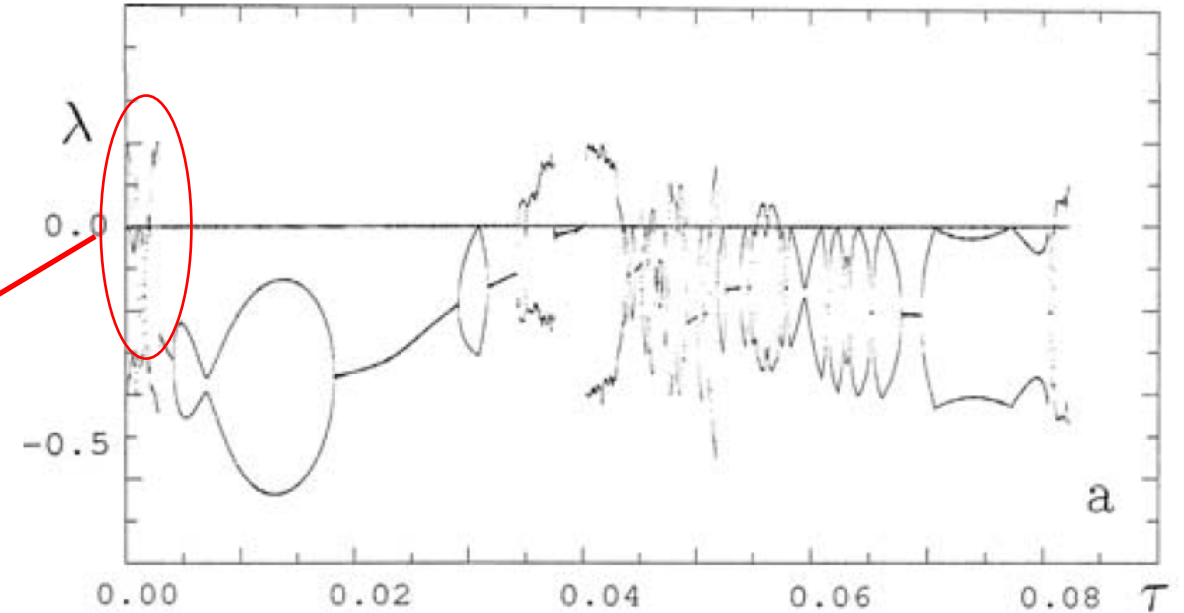
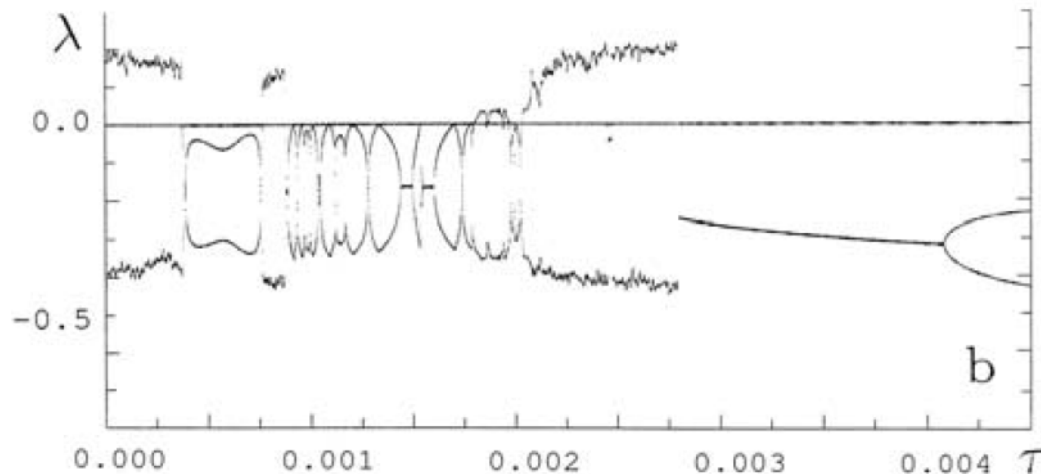
- **Butterfly-effect (Lorenz 1963)**

a tornado (the exact time of formation, the exact path taken) might be influenced by **minor** perturbations such as a distant **butterfly** flapping its wings several weeks earlier.

- **long-term prediction of chaos is impossible !**

Chaos: sensitivity on numerical algorithms

Fully chaotic system



- CP: **Computational Periodicity** (2006)
- CC: **Computational Chaos** (1989)

1. Motivations

Sensitivity on initial condition is physically **acceptable**, since difference of initial condition has physical meanings

Sensitivity on numerical algorithms is physically **unacceptable**, since numerical algorithms are **artificial** factors and have **no** physical meanings at all!

Very pessimistic viewpoint

Teixeira, *et al.* *JOURNAL OF THE ATMOSPHERIC SCIENCES*, 64, 175-189 (2007)

Their main conclusions:

merical convergence. In this paper it is illustrated how, for fully chaotic systems, numerical convergence cannot be guaranteed forever and that for regimes that are not fully chaotic, different time steps may lead to different model climates and even different regimes of the solution.

Intense debate

Tellus

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TELLUS

LETTER TO THE EDITOR

Comment on “Computational periodicity as observed in a simple system,” by Edward N. Lorenz (2006a)

By LUN-SHIN YAO^{1*} and DAN HUGHES², ¹*Mechanical and Aerospace Engineering, Arizona State University, Tempe, AR 85287–6106, USA*, ²*Hughes and Associates, Porter Corners, NY 12859, USA*

(Manuscript received 14 September 2007; in final form 14 November 2007)

ABSTRACT

Systems of ordinary differential equations that exhibit chaotic responses have yet to be correctly integrated. So far no ‘convergent’ computational results have been determined for chaotic differential equations. Various computed numbers are not solutions of the continuous differential equations; all chaotic responses are simply numerical noise and have nothing to do with the solutions of differential equations. It would be an exciting contribution if a convergent computed chaotic solution for a Lorenz model could be obtained.

“It would be an **exciting** contribution if a **convergent** chaotic simulation of Lorenz model is obtained”

“all chaotic responses are simply numerical noises!”

2. Basic ideas of Clean Numerical Simulation (CNS)

- (1) Due to butterfly-effect, numerical noises increases **exponentially**, so that numerical simulations of chaos quickly become a mixture of “**true**” physical solution and “**false**” numerical noises, which are mostly at the **same** order of magnitude.

$$\mathcal{E}(t) = \mathcal{E}_0 \exp(\mu t), \quad t \in [0, T_c],$$

- (2) There exists the so-called “**critical predictable time**” T_c , within it the numerical noises are **negligible** compared to the “**true**” physical solution so that the simulation is **reliable** and “**convergent**” in $0 < t < T_c$.

2. Basic ideas of Clean Numerical Simulation (CNS)

Key problems of the CNS:

- (1) How to determine T_c ?**
- (2) How to enlarge T_c ?**
- (3) How to use CNS results?**

2. Basic ideas of Clean Numerical Simulation (CNS)

Numerical noises
= **maximum**{truncation error, round-off error}

(a) Reduce truncation error:

Time: High-order Taylor expansion

Space: High-order Fourier spectral Method

(b) Reduce round-off error:

multiple-precision with many enough digits

Key point: reduce **both** of truncation and round-off errors!

2. Basic ideas of Clean Numerical Simulation (CNS)

For a given time-step:

$$\mathcal{E}_c = \mathcal{E}_0 \exp(\kappa T_c),$$

$$T_c = \frac{\ln \mathcal{E}_c - \ln \mathcal{E}_0}{\kappa},$$

$$T_c \approx \alpha + \beta N_s,$$

$$T_c \approx \gamma M,$$

$$T_c = \min \left\{ \alpha + \beta N_s, \gamma M \right\}.$$

truncation error \sim round-off error

$$N_s \approx \left[\frac{T_c - \alpha}{\beta} \right] + K_s,$$

$$M \approx \left[\frac{T_c}{\gamma} \right] + K_o,$$

$$N'_s \approx \left[\frac{T_c - T' - \alpha}{\beta} \right] + K_s,$$

$$M' \approx \left[\frac{T_c - T'}{\gamma} \right] + K_o,$$

2. Clean Numerical Simulation



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TELLUS

On the reliability of computed chaotic solutions of non-linear differential equations

By SHIJUN LIAO*, *State Key Laboratory of Ocean Engineering, Shanghai Jiao Tong University,
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(Manuscript received 14 October 2008; in final form 5 March 2009)

2. Basic ideas of Clean Numerical Simulation (CNS)

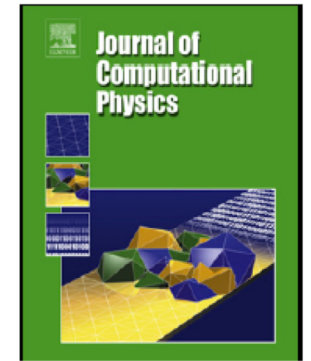
Journal of Computational Physics 418 (2020) 109629



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On the risks of using double precision in numerical simulations of **spatio-temporal chaos**

Tianli Hu^a, Shijun Liao^{a,b,c,d,*}



3. Applications of the CNS

- ① Convergent trajectory of chaotic systems**
- ② Origin of macroscopic randomness**
- ③ Influences of small disturbances to turbulent flow**
- ④ Periodic orbits of three-body systems**

(1) Convergent trajectory of fully chaotic systems

Reliable & convergent chaotic solution of Lorenz EQ

S.J. Liao (2009) : [0,1100]

method: **CNS** order: **M=400** data precision: **N = 800**

P.F. Wang (2011) : [0,2500]

method: **CNS** order: **M=1000** data precision: **N =2100**

B. Kehlet & A. Logg (2013): [0, 1000]

method: **FEM** order : **M=200** data precision : **N=400**

S.J. Liao & P.F. Wang (2013) : [0,10000]

method: **CNS** order: **M=3500** data precision: **N =4180**

It is possible to gain convergent/reliable chaotic result !

(1) Convergent trajectory of chaotic systems

Scientific meanings

- (1) Some **pessimistic** viewpoints such as “**all chaotic responses are simply numerical noises**” (Yao and Hughes), “**for fully chaotic systems, numerical convergence cannot be guaranteed forever**” (Teixeira et al) and so on, are **wrong**.
- (2) Convergent CNS results can be used as **benchmark solutions** to investigate
 - (A) the propagation of micro-level physical uncertainty
 - (B) the influence of numerical noises on statistics of chaos

(2) Origin of macroscopic randomness

Governing equation of 3-body problem:

$$\ddot{x}_{k,i} = \sum_{j=1, j \neq i}^3 \rho_j \frac{(x_{kj} - x_{ki})}{R_{ij}^3}, \quad k = 1, 2, 3,$$

where

$$R_{ij} = \left[\sum_{k=1}^3 (x_{kj} - x_{ki})^2 \right]^{1/2}$$

and

$$\rho_i = \frac{m_i}{m_1}, \quad i = 1, 2, 3$$

denotes the ratio of the mass.

Initial conditions:

$$\mathbf{r}_1 = (0, 0, -1) \quad \mathbf{r}_2 = (0, 0, 0), \quad \mathbf{r}_3 = -(\mathbf{r}_1 + \mathbf{r}_2),$$

$$\dot{\mathbf{r}}_1 = (0, -1, 0), \quad \dot{\mathbf{r}}_2 = (1, 1, 0), \quad \dot{\mathbf{r}}_3 = -(\dot{\mathbf{r}}_1 + \dot{\mathbf{r}}_2),$$

Body 1 & 3

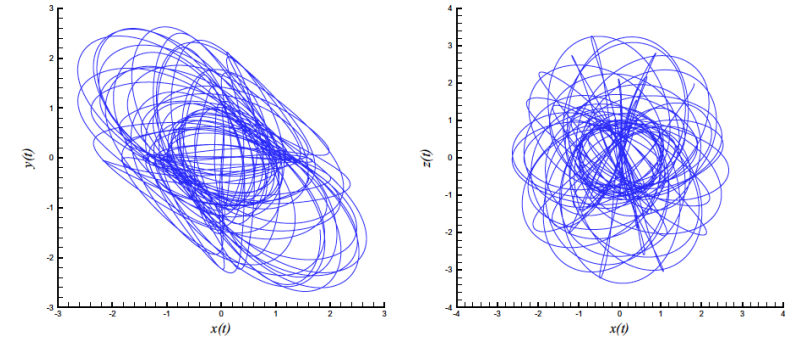


Fig. 2. x - y and x - z of Body 1 ($0 \leq t \leq 1000$) in the case of $\delta = 0$.

Body-2

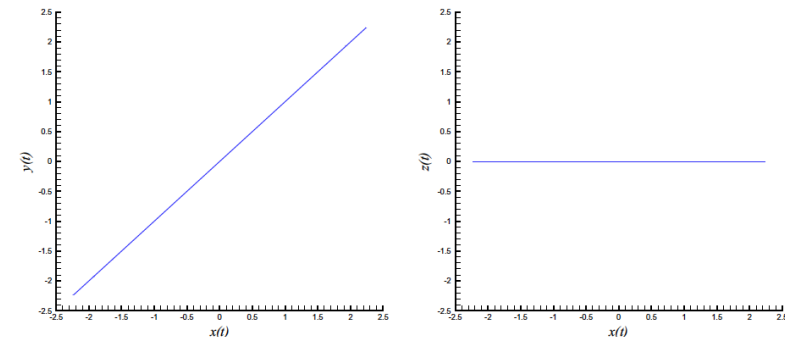


Fig. 3. x - y and x - z of Body 2 ($0 \leq t \leq 1000$) in the case of $\delta = 0$.

(2) origin of macroscopic randomness

$$\dot{\mathbf{r}}_1 = (0, -1, 0), \dot{\mathbf{r}}_2 = (1, 1, 0), \dot{\mathbf{r}}_3 = -(\dot{\mathbf{r}}_1 + \dot{\mathbf{r}}_2),$$

Uncertainty of position:

Initial position: $\mathbf{r}_1 = (0, 0, -1) + \delta(1, 0, 0),$
 $\mathbf{r}_2 = (0, 0, 0), \quad \mathbf{r}_3 = -(\mathbf{r}_1 + \mathbf{r}_2)$

Three cases:

$$(1) \delta = 0 \quad (2) \delta = +10^{-60} \quad (3) \delta = -10^{-60}$$

This uncertainty is **less** than Planck length $1.62\text{E-}35$ m, and thus is negligible in physics, say, the **same** initial conditions **in physics**!

Trajectory of Body-1

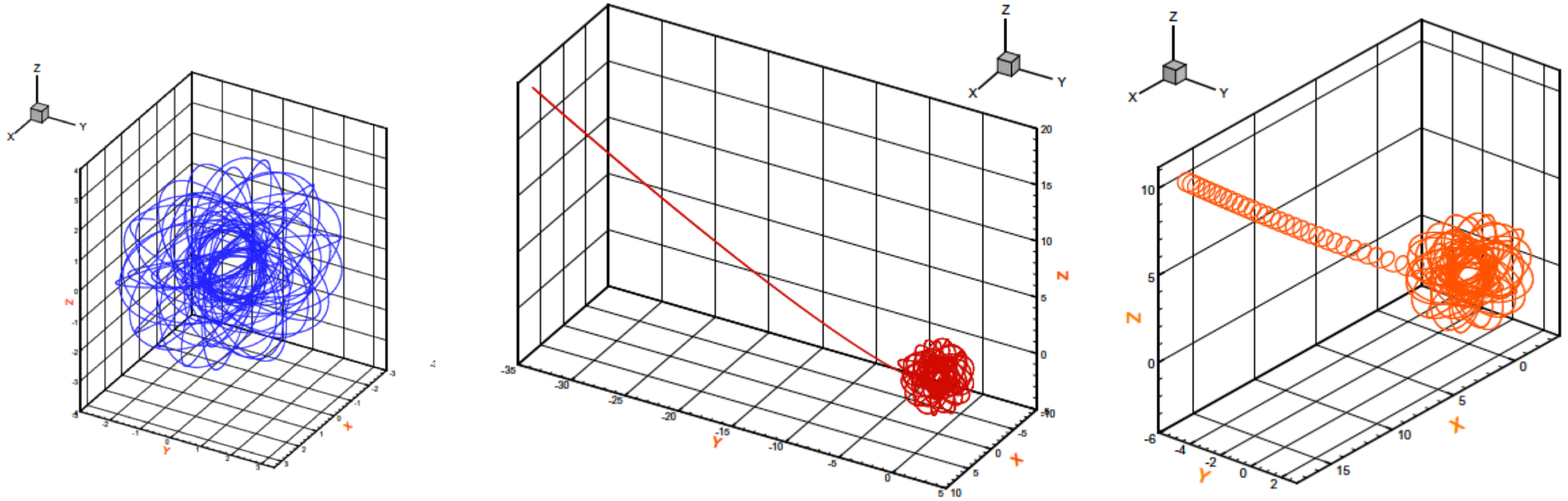


Fig. 12. Orbit of Body 1 ($0 \leq t \leq 1000$). Left: $\delta = +10^{-60}$; Right: $\delta = -10^{-60}$.

$$\delta = 0$$

$$\delta = 10^{-60}$$

$$\delta = -10^{-60}$$

Trajectory of Body-2

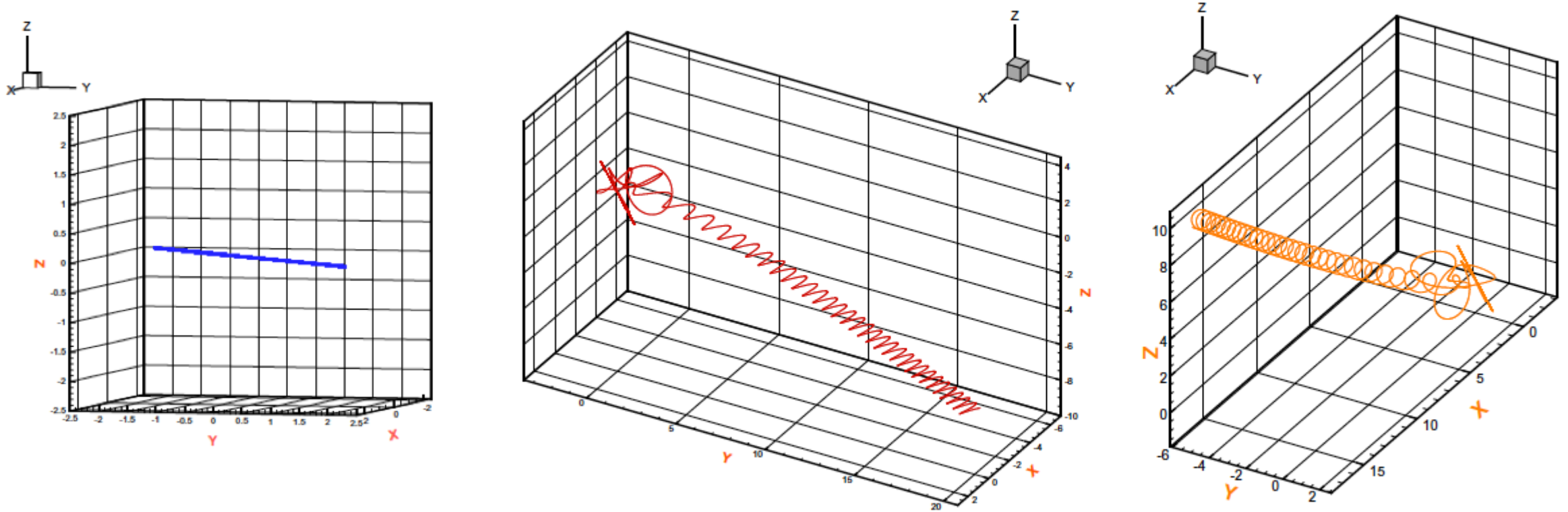


Fig. 13. Orbit of Body 2 ($0 \leq t \leq 1000$). Left: $\delta = +10^{-60}$; Right: $\delta = -10^{-60}$.

$$\delta = 0$$

$$\delta = 10^{-60}$$

$$\delta = -10^{-60}$$

Trajectory of Body-3

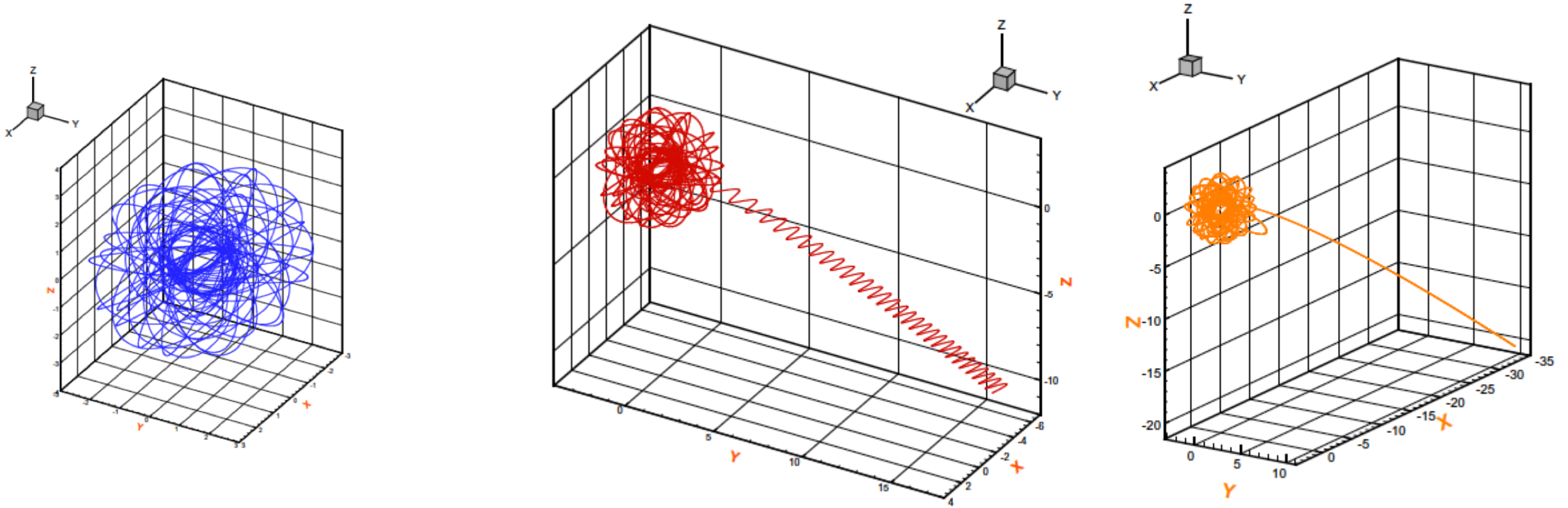


Fig. 14. Orbit of Body 3 ($0 \leq t \leq 1000$). Left: $\delta = +10^{-60}$; Right: $\delta = -10^{-60}$.

$$\delta = 0$$

$$\delta = 10^{-60}$$

$$\delta = -10^{-60}$$

(2) origin of macroscopic randomness

$$\mathbf{r}_i(0) = \bar{\mathbf{r}}_i(0) + \mathbf{r}'_i(0), \quad \bar{\mathbf{r}}_i(0) = \langle \mathbf{r}_i(0) \rangle \quad \langle \mathbf{r}'_i(0) \rangle = 0 \quad \text{and} \quad \sqrt{\langle \mathbf{r}'_i{}^2(0) \rangle} = \sigma_0.$$

$$\bar{\mathbf{r}}_1 = (0, 0, -1), \quad \bar{\mathbf{r}}_2 = (0, 0, 0), \quad \bar{\mathbf{r}}_3 = -(\bar{\mathbf{r}}_1 + \bar{\mathbf{r}}_2),$$

$$\dot{\mathbf{r}}_1 = (0, -1, 0), \quad \dot{\mathbf{r}}_2 = (1, 1, 0), \quad \dot{\mathbf{r}}_3 = -(\dot{\mathbf{r}}_1 + \dot{\mathbf{r}}_2).$$

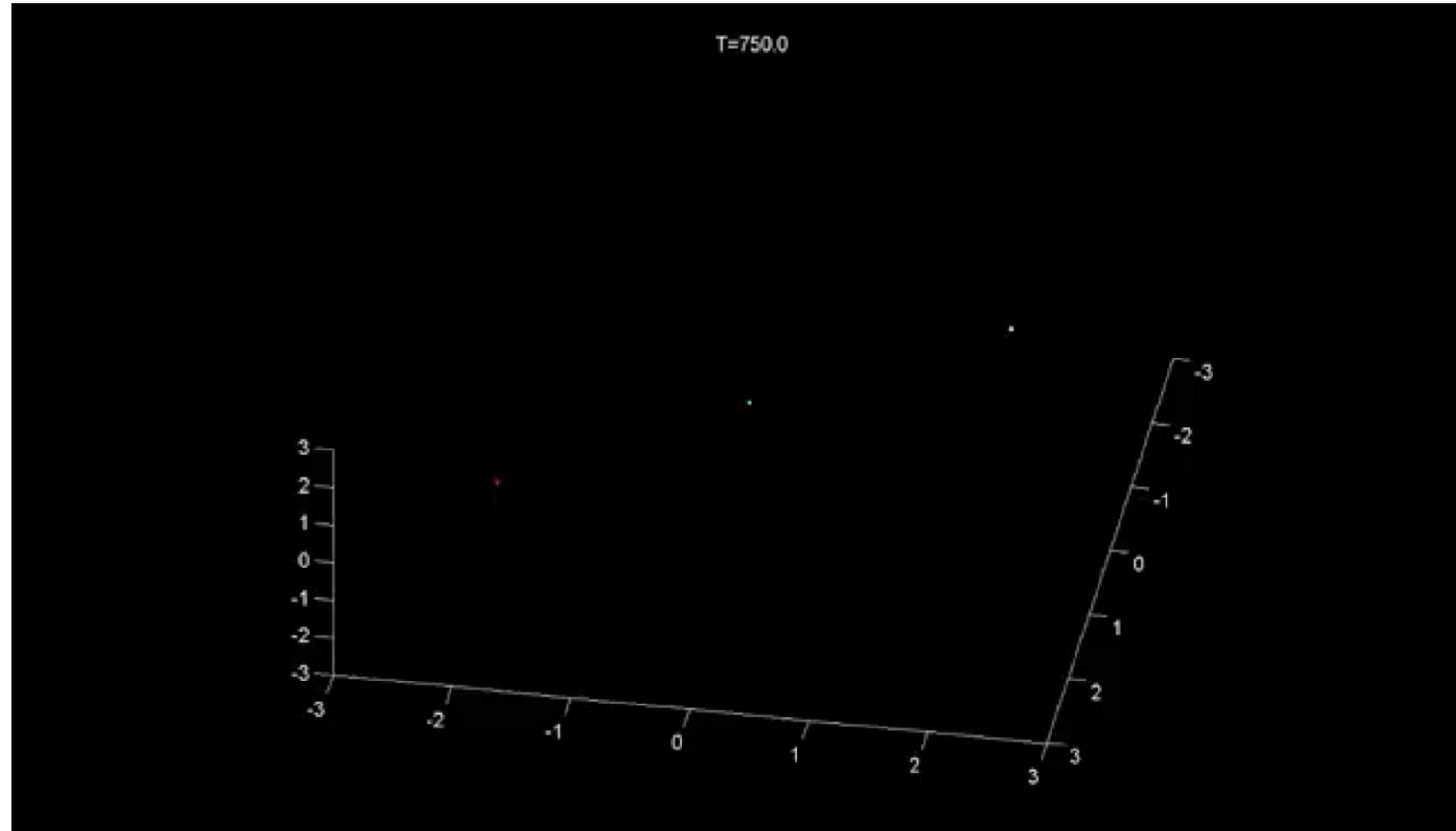
$$\text{Variance : } \sigma_0 = 10^{-60}$$

10000 samples:

Body-1: red

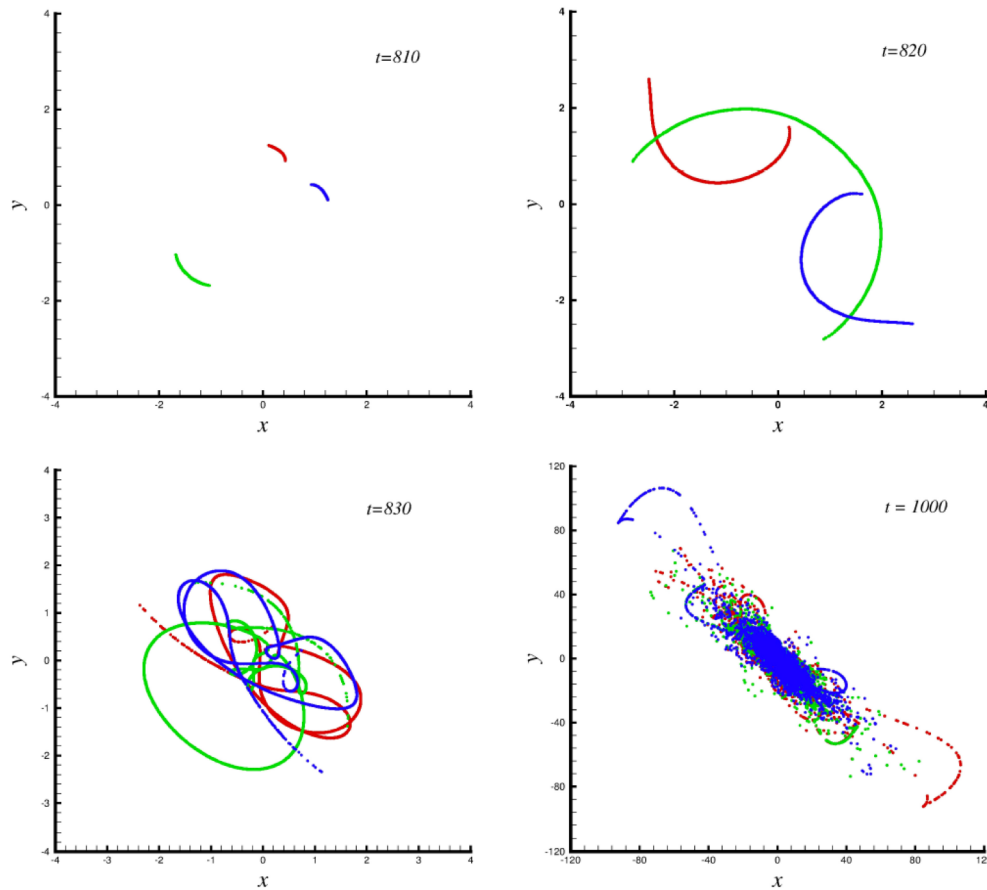
Body-2: yellow

Body-3: blue

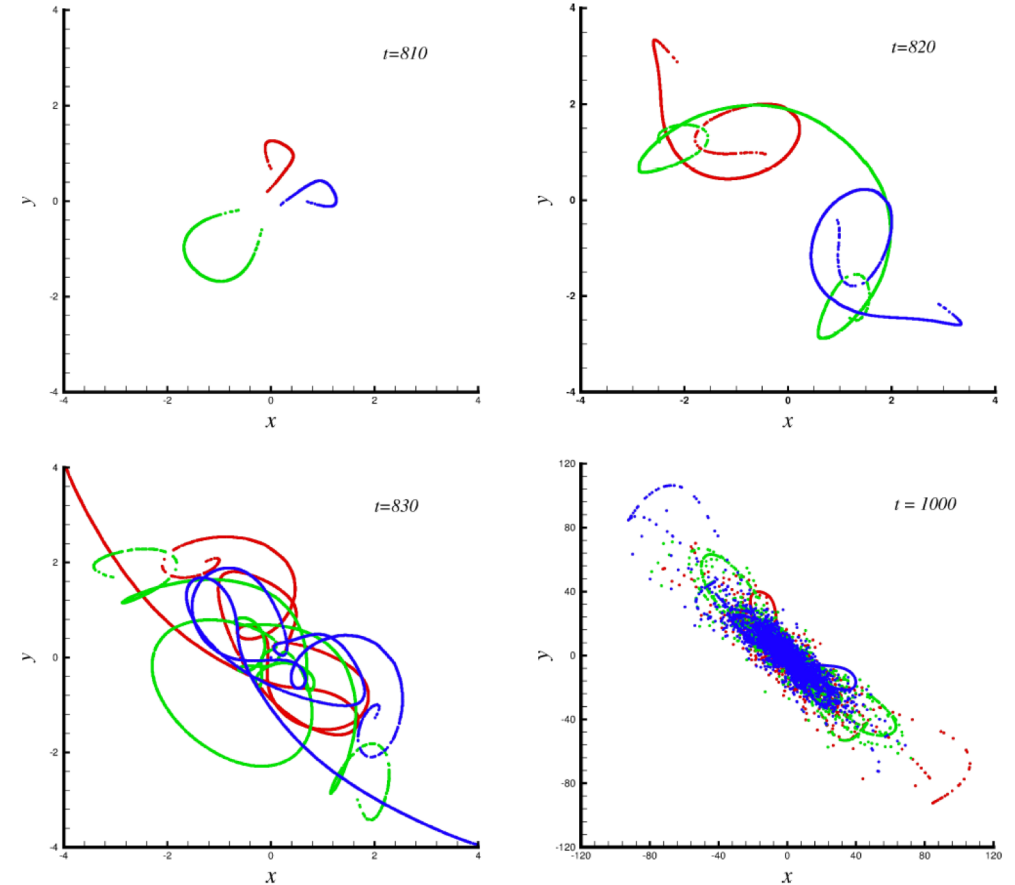


Statistic sensitivity to micro-level uncertainty

$$\sigma_0 = 10^{-60}$$



$$\sigma_0 = 3 \times 10^{-60}.$$



(2) Origin of macroscopic randomness

- **micro-level** uncertainty might be an **origin** of some **macroscopic** uncertainty
- **Macroscopic** statistics are **sensitive** to statistics of **micro-level** uncertainty
- **escape** and **symmetry breaking** of 3-body system are **self-excited** **without** any external disturbances
- an universe could **randomly** evolve by **itself** into complicated structures, **without** any external forces.

(3) Influence of small disturbances to turbulence

J. Fluid Mech. (2022), vol. 948, A7, doi:10.1017/jfm.2022.710

JM PAPERS



Large-scale influence of numerical noises as artificial stochastic disturbances on a sustained turbulence

Shijie Qin¹ and Shijun Liao^{1,2,†}

(3) Influence of small disturbances to turbulence

Two types of Rayleigh–Bénard flows

(a) typical vortical / roll-like flow

(b) zonal flow

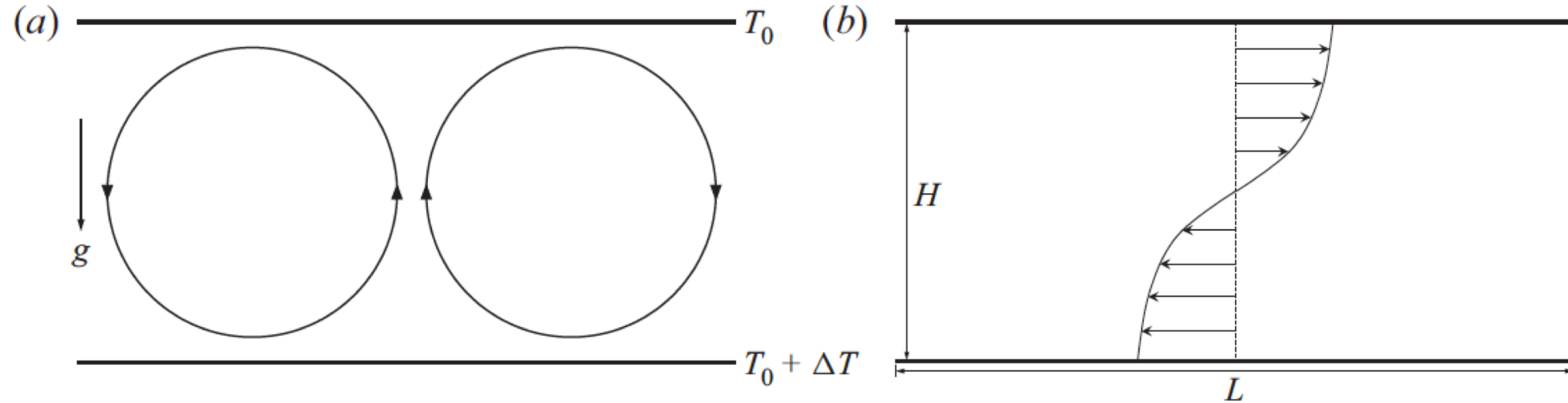


Figure 1. Schematic drawings of 2-D turbulent RBC in two totally different flow types: (a) typical vortical/roll-like flow, and (b) zonal flow. The fluid layer between two parallel plates that are separated by a height H obtains heat from the bottom boundary surface because of the constant temperature difference $\Delta T > 0$, where L is the horizontal length of the computational domain, and the downward direction of gravity acceleration g is indicated.

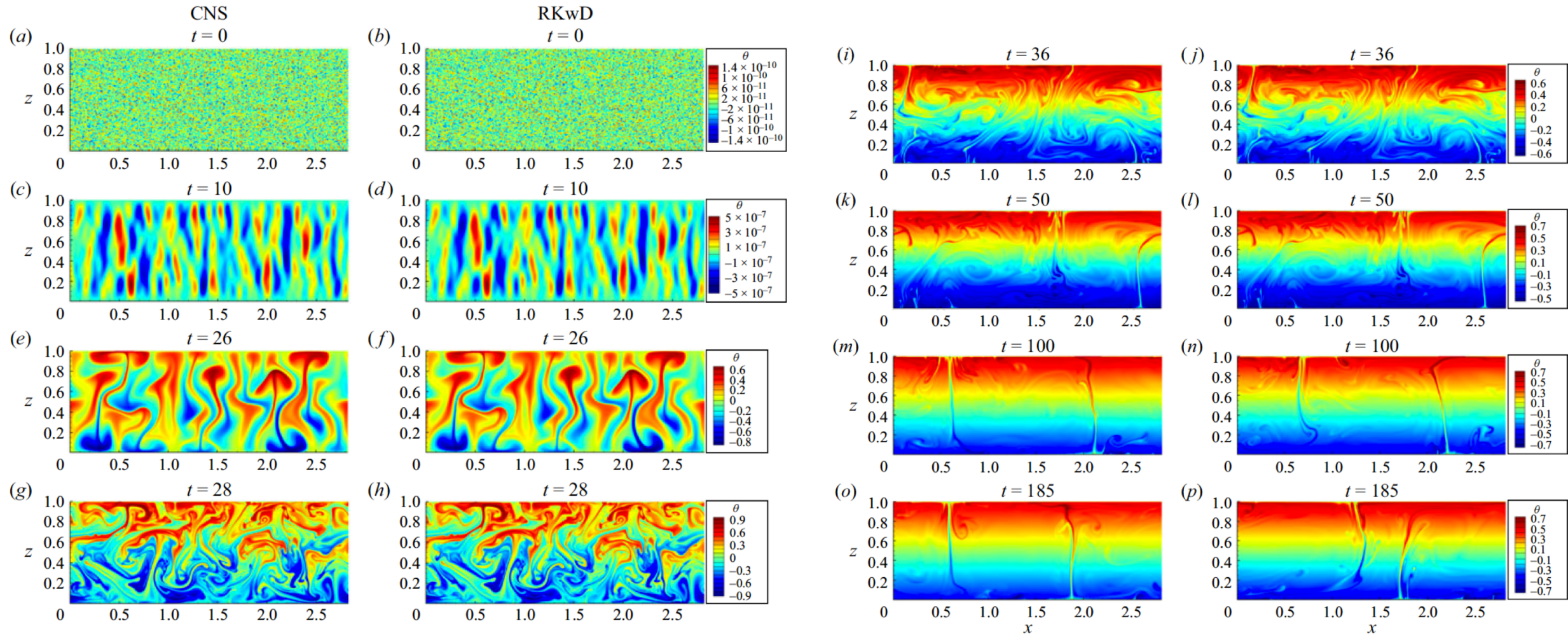
(3) Influence of small disturbances to turbulence

The NS equations with the **same** initial/boundary condition and the **same** physical parameters are solved by means of the **DNS with double precision** and the **CNS with multiple precision**.

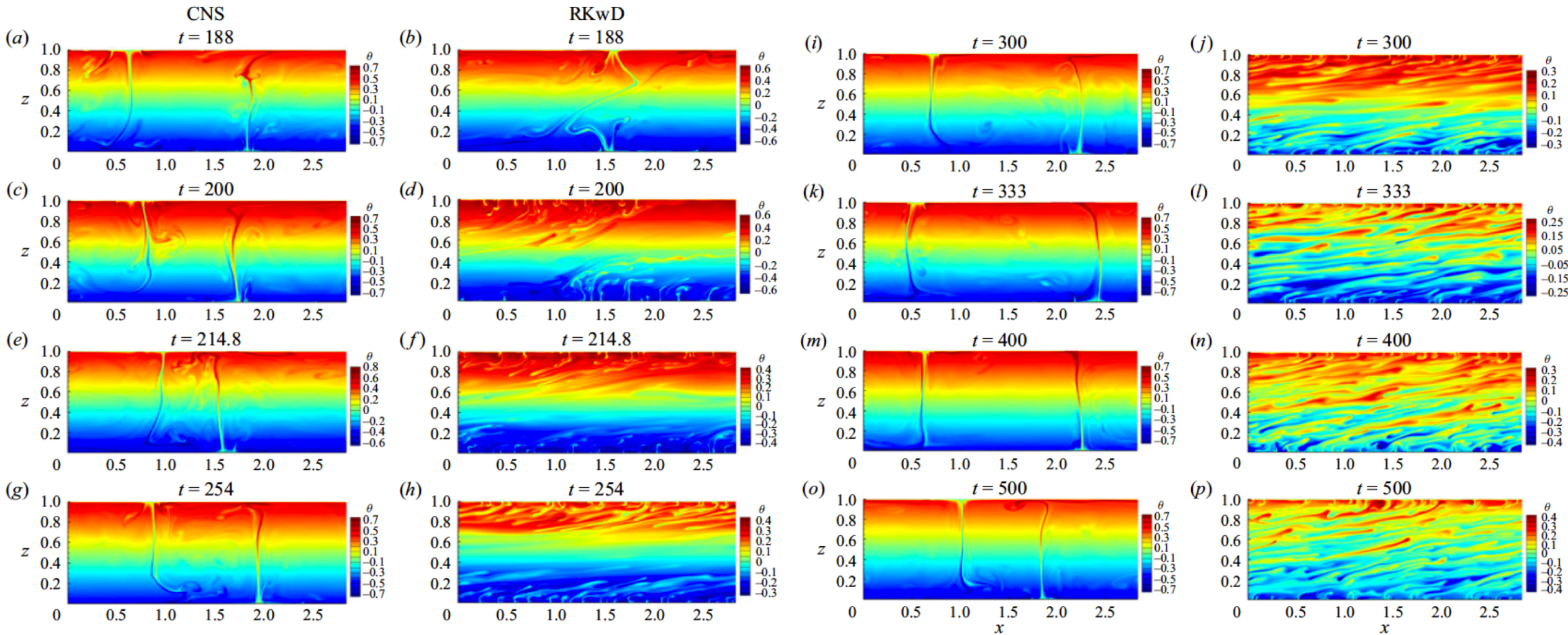
CNS: **always** typical vortical/roll-like flow

DNS: **first** typical vortical/roll-like flow, **but then** zonal flow

(3) Influence of small disturbances to turbulence



(3) Influence of small disturbances to turbulence



(3) Influence of small disturbances to turbulence

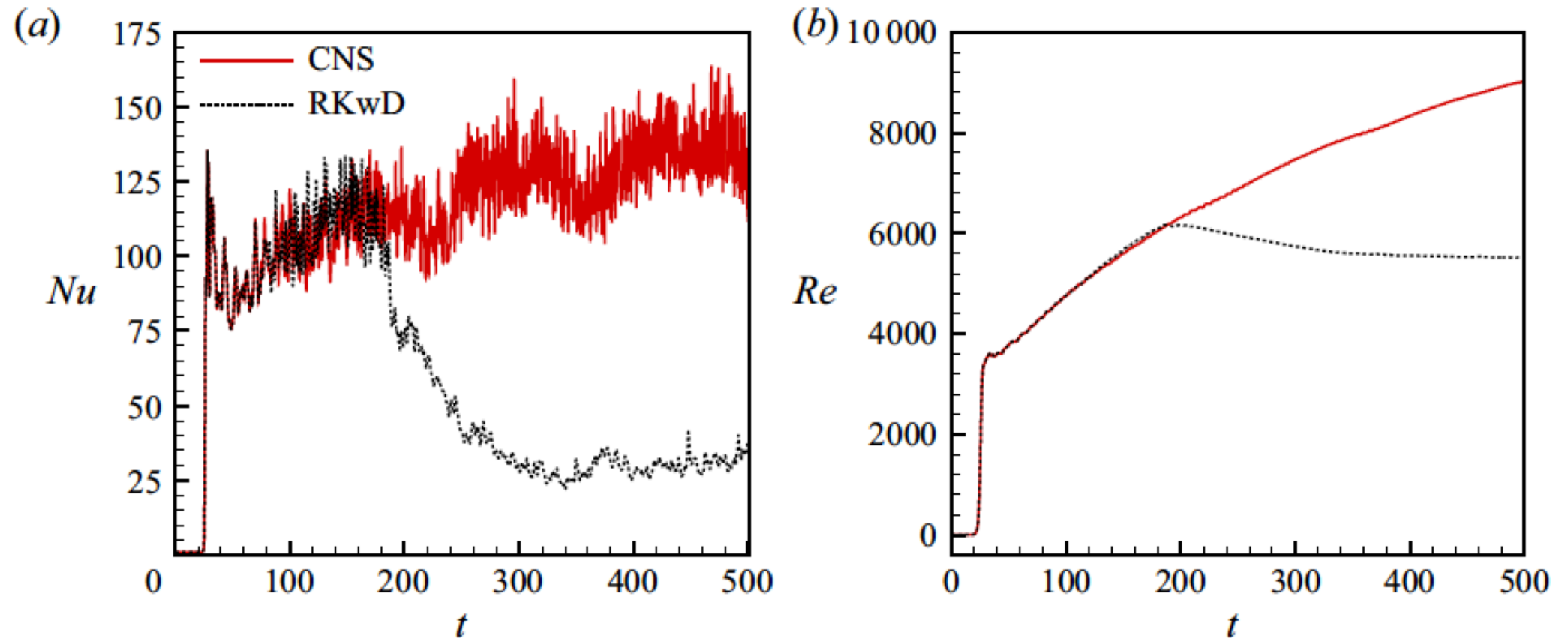
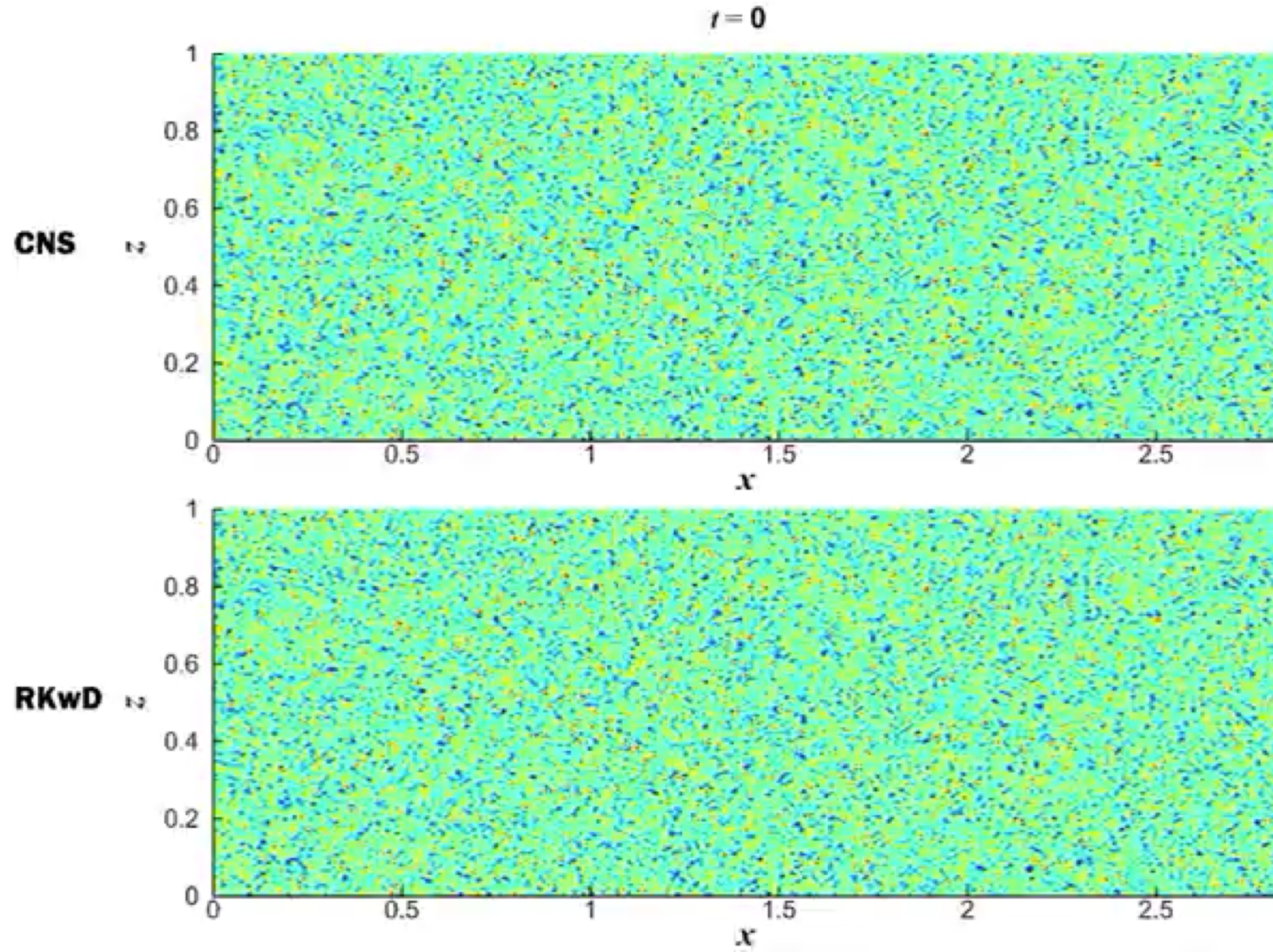


Figure 4. Comparisons of the instantaneous Nusselt number Nu and Reynolds number Re in the case $Pr = 6.8$, $Ra = 6.8 \times 10^8$ and $L/H = 2\sqrt{2}$: (a) the Nusselt number Nu ; (b) the Reynolds number Re . Solid line in red denotes the CNS benchmark solution; dashed line in black denotes the RKwD simulation using $\Delta t = 10^{-4}$.

(3) Influence of small disturbances to turbulence

Numerical noises have
quantitatively and qualitatively
large-scale
influences on a
sustained
turbulence!



Chaos = normal-chaos + ultra-chaos

- **Normal-chaos:** whose statistics is **stable** to small disturbances
- **Ultra-chaos:** whose statistics is **sensitive** to small disturbances

Advances in Applied Mathematics and Mechanics
Adv. Appl. Math. Mech., Vol. 14, No. 4, pp. 799-815

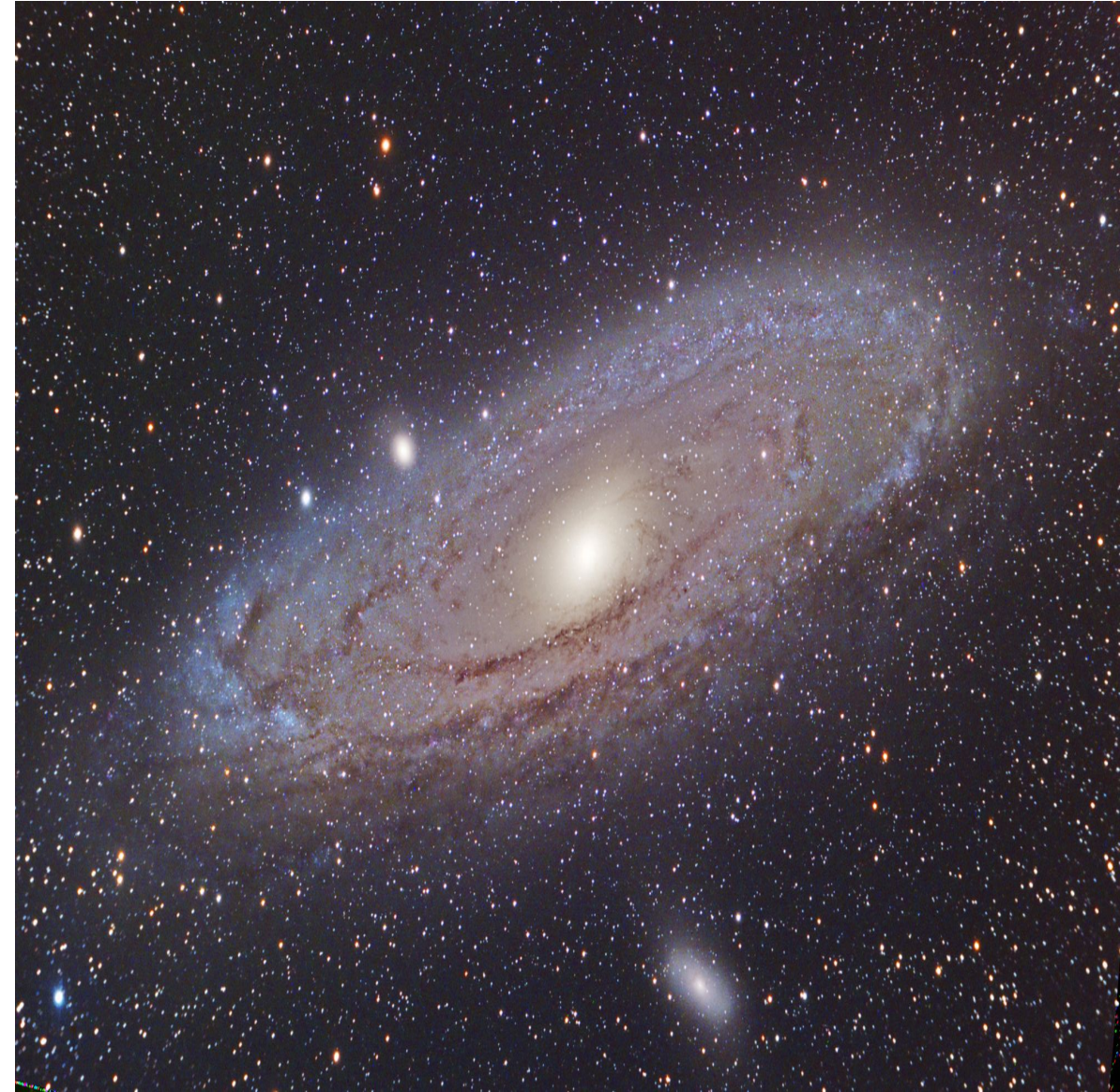
DOI: 10.4208/aamm.OA-2021-0364
August 2022

Ultra-Chaos: an Insurmountable Objective Obstacle of Reproducibility and Replication

Shijun Liao^{1,2,3,*} and Shijie Qin²

(4) New periodic orbits of 3-body problem

1. Are there living beings **outside** of earth?
2. Stable periodic planets can provide a stable **space-time** background for **evolution** of living beings



(4) New periodic orbits of 3-body problem

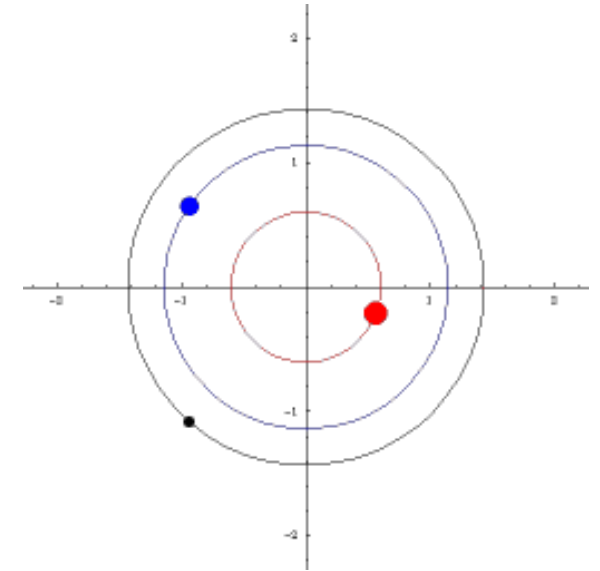
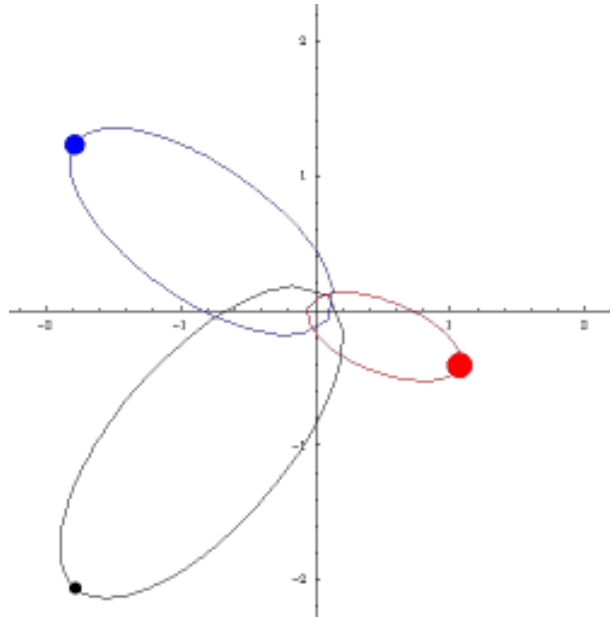
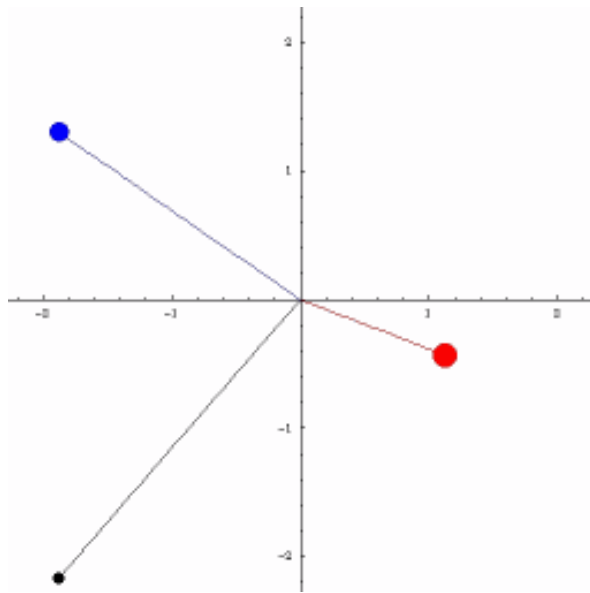


Scientists who have studied the three-body problem (clockwise from left): Newton, Euler, Poincaré, Laplace, Lagrange

1. The 3-body problem was proposed by Newton (1687)
2. Many mathematicians and physicists, such as **Euler**, **Lagrange**, **Laplace**, **Poincaré**, and **Hilbert**, have studied it
3. It is still an open question

(4) New periodic orbits of 3-body problem

Euler (1767) and Lagrange (1772) :



According to Chenciner and Montgomery (2000) in *Annals of Mathematics*, only **three** family of periodic orbits of three-body problem with **3 equal mass** were found in 300 years after Newton!

Why is it so difficult ?

Poincaré (1890) :

(A) The uniform first integral does **not exist in general. Thus, one **had to** use numerical methods to gain periodic orbits**

(B) **Butterfly-effect:
extremely sensitive to the initial conditions**

Founder of “Chaotic Dynamics**”**



**Poincaré
(1854-1912)**

M. Suvakov and V. Dmitrasinovic, Phys. Rev. Lett. 110, 114301 (2013).

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Physicists Discover a Whopping 13 New Solutions to Three-Body Problem

By Jon Cartwright | Mar. 8, 2013 , 4:30 PM

Why so few were found ? Supercomputer + ?

(4) New periodic orbits of 3-body problem

New strategy: supercomputer + **CNS**

1. Guarantee that trajectories of three-body problems are **convergent/reliable** in a long enough interval of time by the CNS
2. Find some candidates by grid search method
3. Modify the initial conditions of these candidates by Newton-Raphson

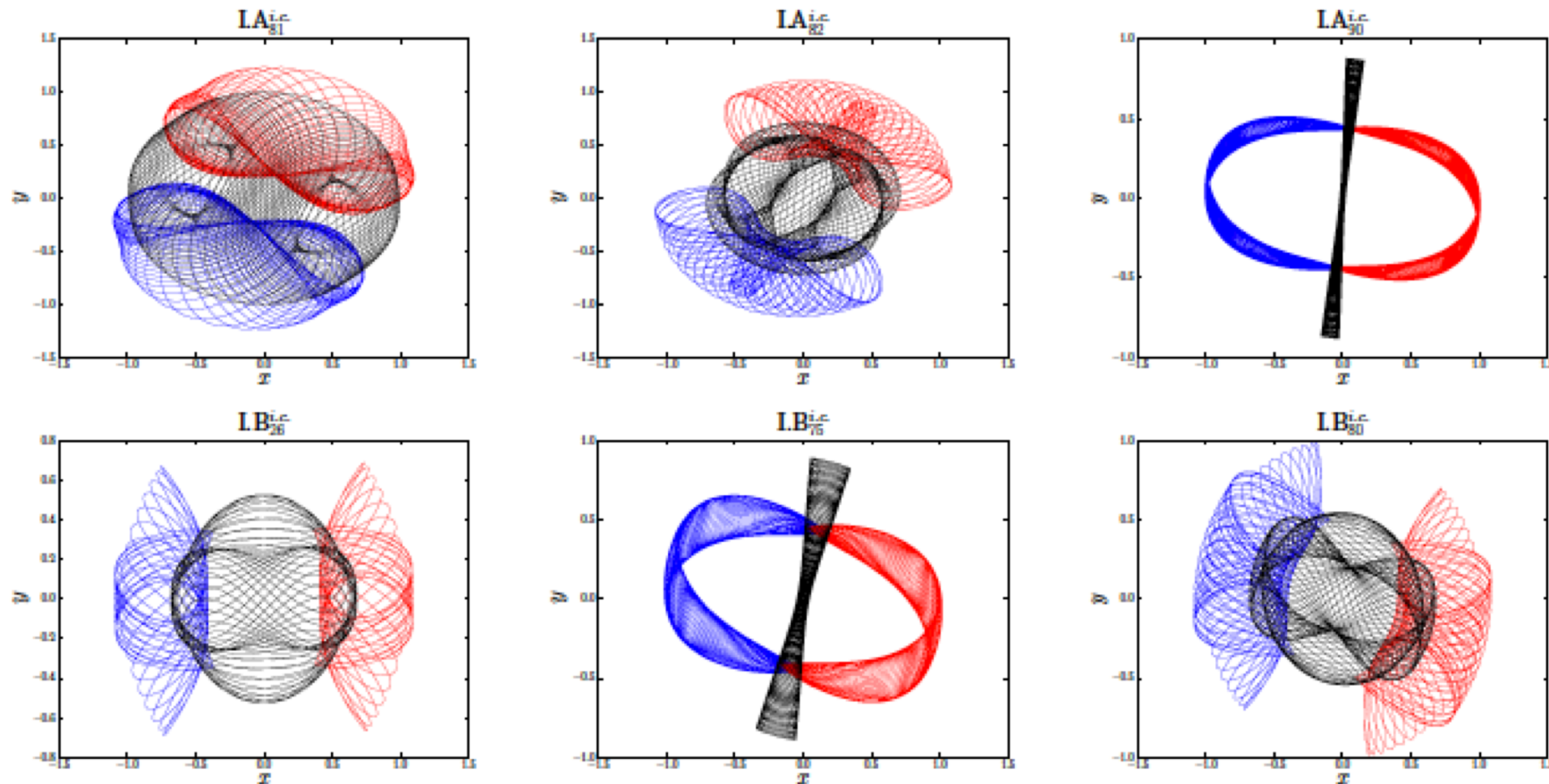
Published papers

1. X.M. Li and S.J. Liao, “More than six hundred new families of Newtonian periodic planar collisionless three-body orbits”, *Science China - Physics Mechanics & Astronomy*, Vol. 60, No. 12, 129511 (2017)
2. X.M. Li, Y.P. Jing and S.J. Liao, “Over a thousand new periodic orbits of planar three-body system with unequal mass”, *Publications of Astronomical Society of Japan*, 70 (4), 64 (1–7) (2018)
3. X.M. Li and S.J. Liao, “Collisionless periodic orbits in the free-fall three-body problem”, *New Astronomy*, vol. 70, pp. 22-26 (2019)
4. X.M. Li and S.J. Liao, “One family of 13315 stable periodic orbits of the non-hierarchical unequal-mass triple system”, *Science China – Physics, Mechanics & Astronomy* vol. 64, 219511 (2021)
5. Shijun Liao, Xiaoming Li and Yu Yang, “Three-body problem: from Newton to supercomputer plus machine learning”, *New Astronomy* 96 (2022) 101850.

<http://numericaltank.sjtu.edu.cn/three-body/three-body.htm>

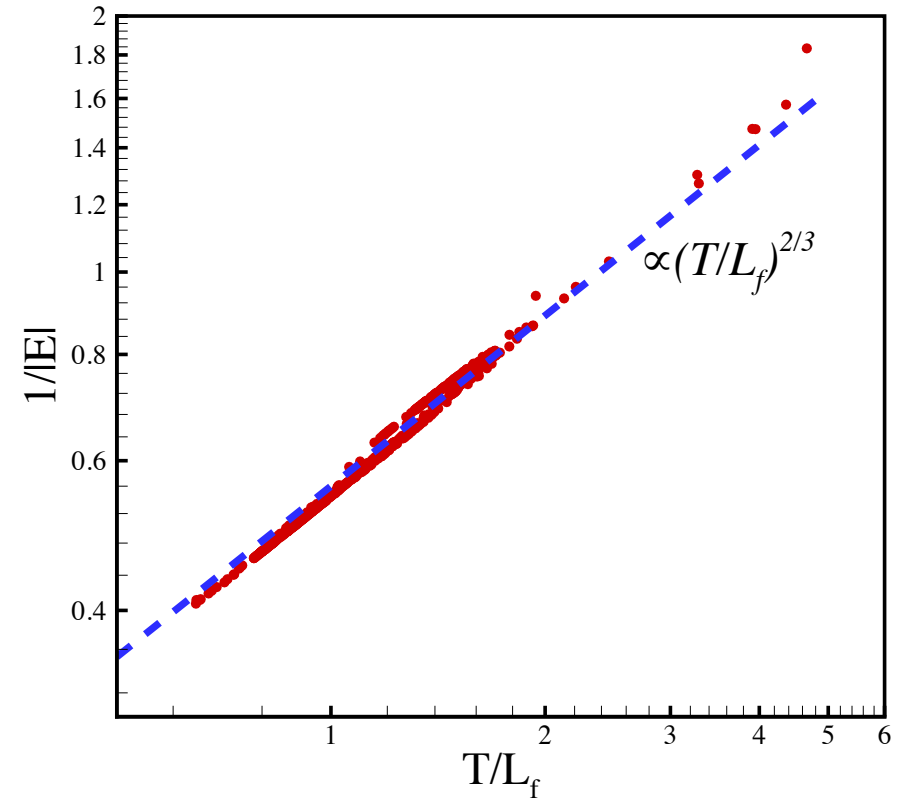
(a) Periodic orbits of 3-body with **three** equal masses

<http://numericaltank.sjtu.edu.cn/three-body/three-body.htm>



(a) Periodic orbits of 3-body with **three** equal masses

**A generalized Kepler law
was found !**



They all satisfy a generalized Kepler law !

(c) Road map for periodic orbits with arbitrary mass

New Astronomy 96 (2022) 101850



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Three-body problem — From Newton to supercomputer plus machine learning

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^c School of Physics and Astronomy, Shanghai Jiaotong University, Shanghai 200240, China

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^e MOE Key Laboratory of Disaster Forecast and Control in Engineering, Guangzhou 510632, China

(c) Road map for periodic orbits with arbitrary mass

Using **machine learning** to predict a good approximation **of initial guess** and applying the **CNS** to **gain convergent trajectory**, we propose a **road map** to gain periodic orbits of three-body system with **arbitrary** masses

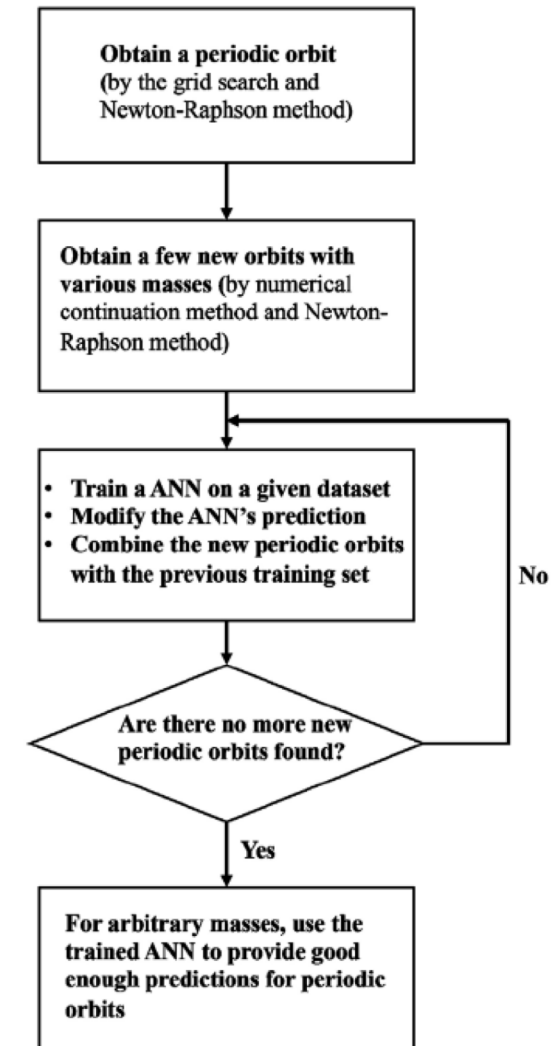


Fig. 9. A roadmap for searching the periodic orbits of three-body problem.

(c) Road map for periodic orbits with arbitrary mass

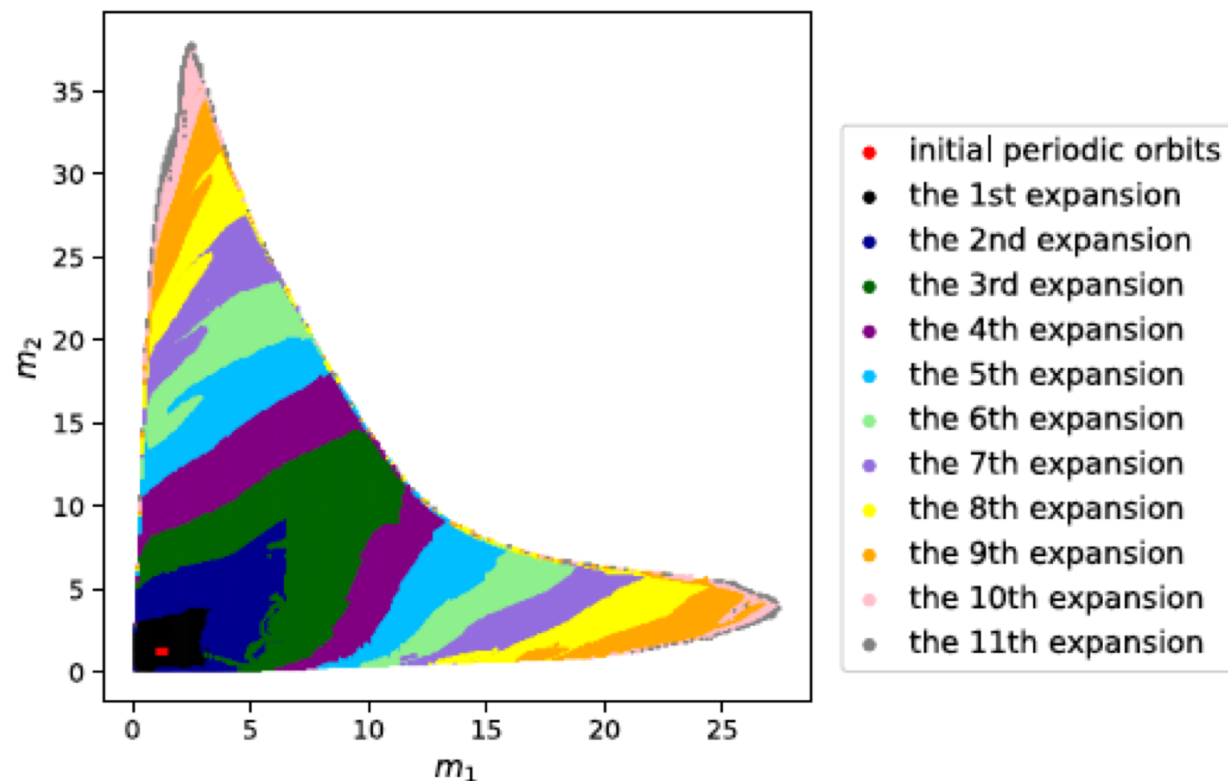


Fig. 5. The relatively periodic orbits with the same rotation angle $\theta = 0.0105056462558377$ of reference frame, found in each extrapolation/expansion on the various mass regions. Red dot: initial periodic orbits; black dot: 1st expansion; dark blue dot: 2nd expansion; dark green dot: the 3rd expansion; dark purple dot: the 4th expansion; light blue dot: the 5th expansion; light green dot: the 6th expansion; light purple dot: the 7th expansion; yellow dot: the 8th expansion; orange dot: the 9th expansion; pink dot: the 10th expansion; gray dot: the 11th expansion.

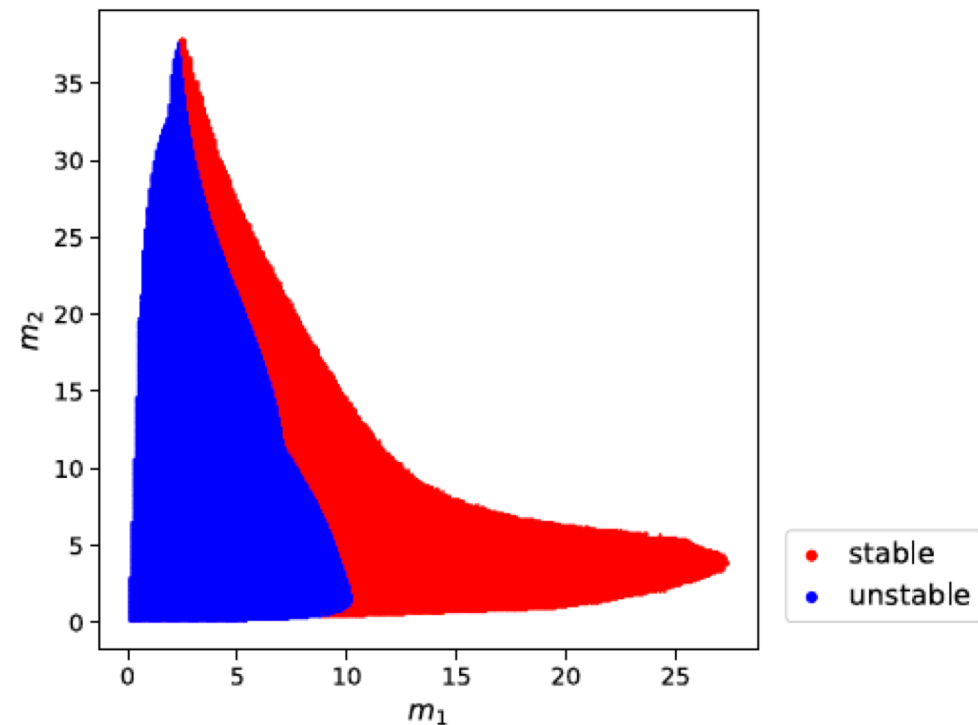
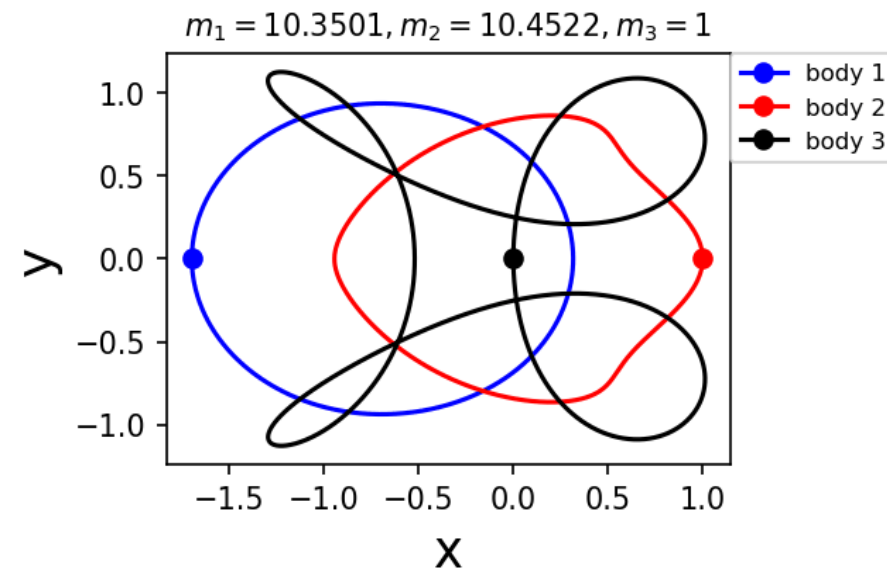
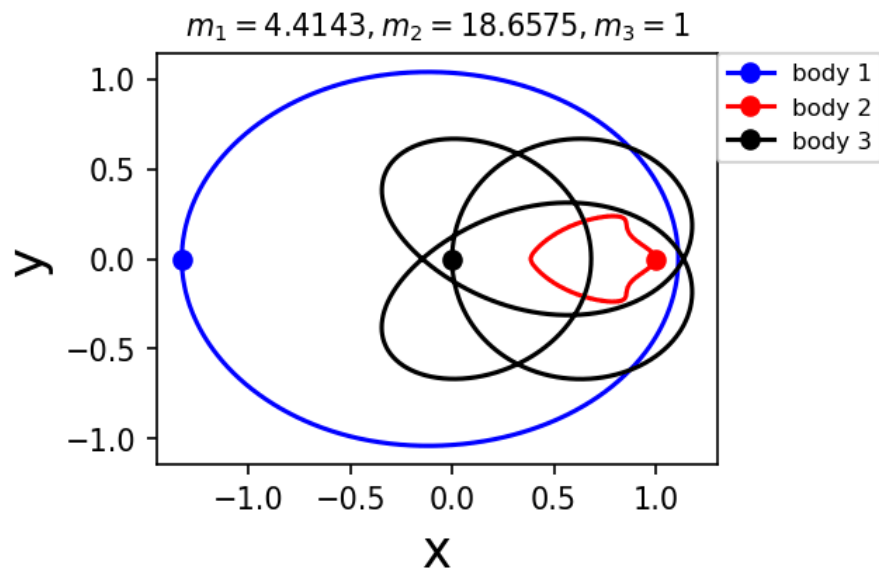
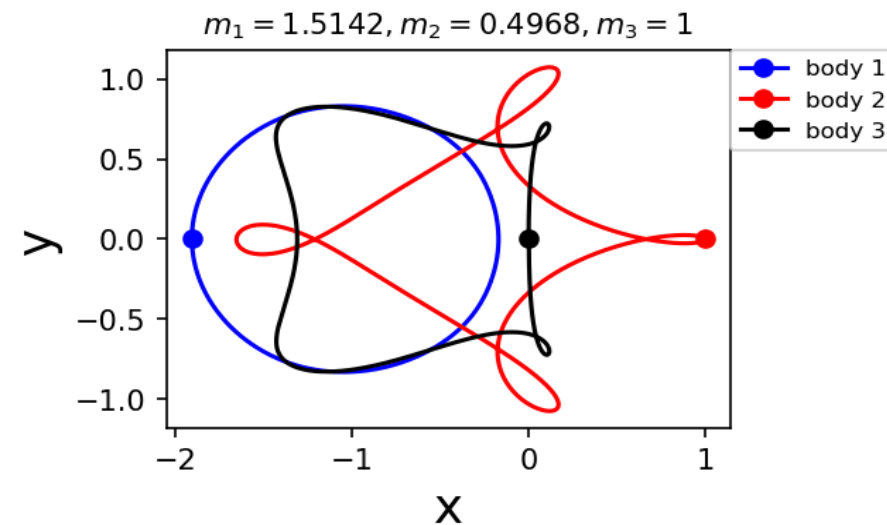
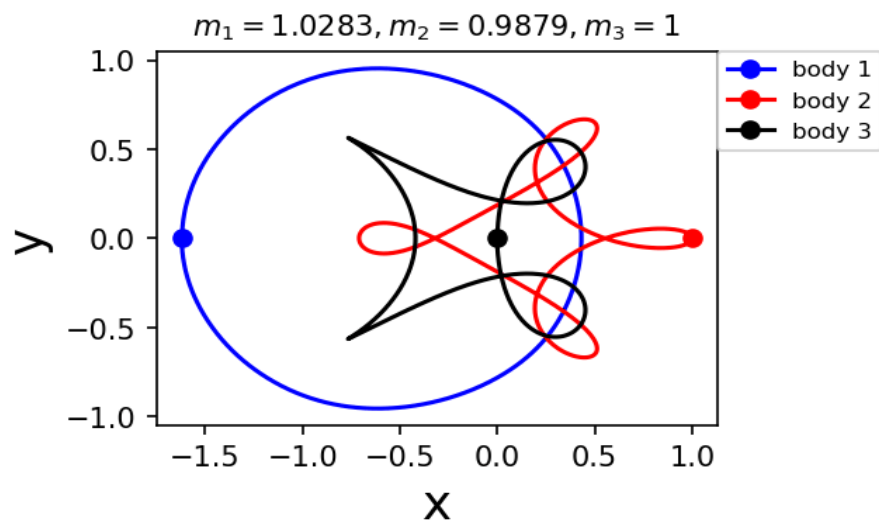


Fig. 7. The linear stability of the relatively periodic orbits in the second case with the rotation angle $\theta = 0.0105056462558377$. Red domain: stable; blue domain: unstable.

(s) Road map for periodic orbits with arbitrary mass



New strategy: supercomputer + CNS + AI

Roadmap

- Xiaoming Li and Liao (2017):
Three equal masses : 695 families of periodic orbits,
more than 600 are totally new
- Xiaoming Li, Yipeng Jing & Shijun Liao (2017):
Two equal masses : 1349 families of new periodic orbits
- Xiaoming Li, X.C. Li & Shijun Liao (2020):
Arbitrary masses : From a known periodic orbit of 3-body problem,
new periodic orbits with various masses can be obtained.
For example, we obtained 135445 new unequal masses periodic solutions.
- Shijun Liao, Xiaoming Li & Yu Yang (2022):
A road map to gain periodic orbits with arbitrary mass by means of AI



The discovery of new orbits were reported **twice** by **New Scientists**

NewScientist



DAILY NEWS 20 September 2017

Infamous three-body problem has over a thousand new solutions



So many possibilities
DeAgostini/Getty

By Leah Crane

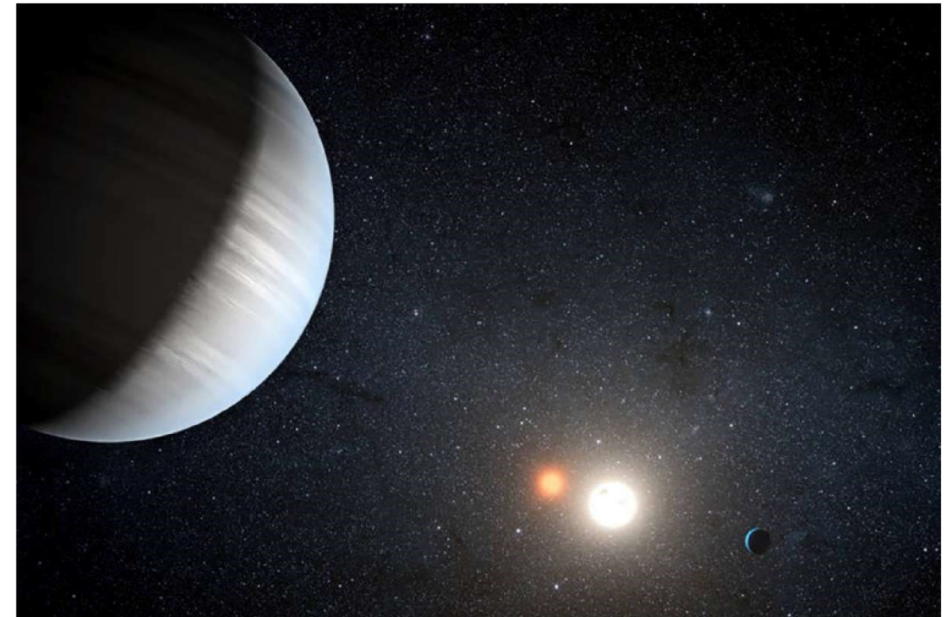
For more than 300 years, mathematicians have puzzled over the three-body problem – the question of how three objects orbit one another according to Newton's laws. Now, there are

NewScientist



DAILY NEWS 25 May 2018

Watch the weird new solutions to the baffling three-body problem



It takes three to tango
NASA/JPL-CalTech/T. Pyle

By Chelsea Whyte

The infamous three-body problem – the mathematical puzzle of how three objects can orbit one another according to Newton's laws – now has hundreds of new solutions.

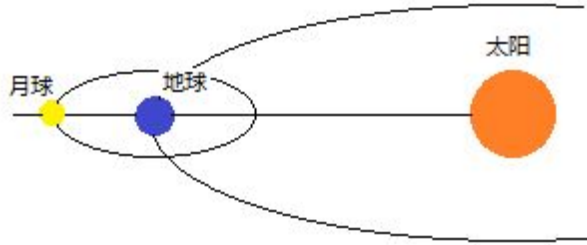
Last year, **Shijun Liao at Shanghai Jiaotong University in China and his colleagues** used a supercomputer to calculate more than a thousand new solutions, nearly doubling the known

Scientific meanings

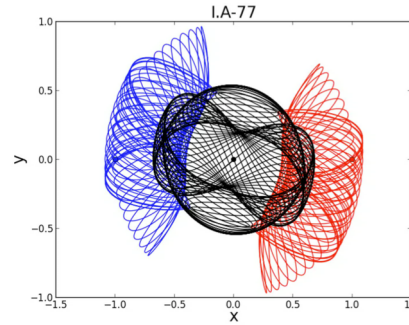
1. Propose a **new strategy** : supercomputer + **CNS**
2. Increases the number of periodic orbits by **several orders** of magnitude
3. Propose an **effective roadmap**: from three/two **equal** masses to **arbitrary** masses

Scientific meanings

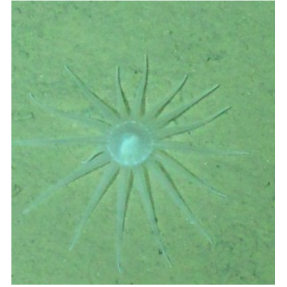
hierarchical :



non-hierarchical :



马里亚纳海沟 海底生物



- Michel Mayor and Didier Queloz won the 2019 Nobel Prize in Physics for discovering the first planet (**hierarchical structure**) orbiting a sun-like star outside the solar system.

Michel Mayor



Didier Queloz

It is expected that some **non-hierarchical** planets can be actually **observed** in the future.

A short Review

- Newton (1687): the three-body problem proposed
- Euler (1767): a closed-form solution (collinear)
- Lagrange (1772): a closed-form solution (equivalence)
- Poincare (1890): Non-existence of first integral
Founder of “Chaos Dynamics”
- BHH (1970s): BHH periodic solution (computer)
- Moore (1993): periodic solution “figure-8” (computer)
- Suvakov et al. (2013): 11 new periodic solution (computer)
- Li, Jing & Liao : 2035 new periodic solutions
(2017) (computer + CNS)
- LI & Liao : 135445 new periodic solutions
(2020) (computer + CNS)
- Liao, Li and Yang A road map for 3-body problem
(2022) (computer + CNS + AI)

Our **strategy** and **roadmap** for finding the periodic solutions to three-body problem work **quite well** !

Today, nothing can prevent human beings from obtaining massive periodic solutions of three-body problem. This is due to the great contributions of some great mathematicians, scientists and engineers in more than three hundred years!



Newton
(1642-1727)



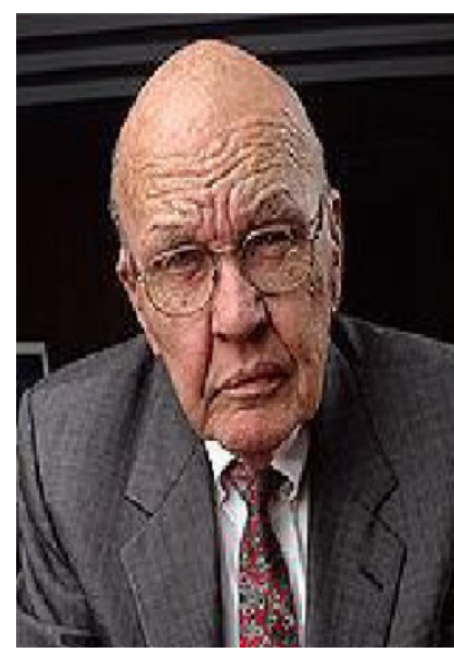
Poincaré
(1854-1912)



Turing
(1912-1954)



Von Neumann
(1903-1957)



Jack Kilby
(1923-2005)

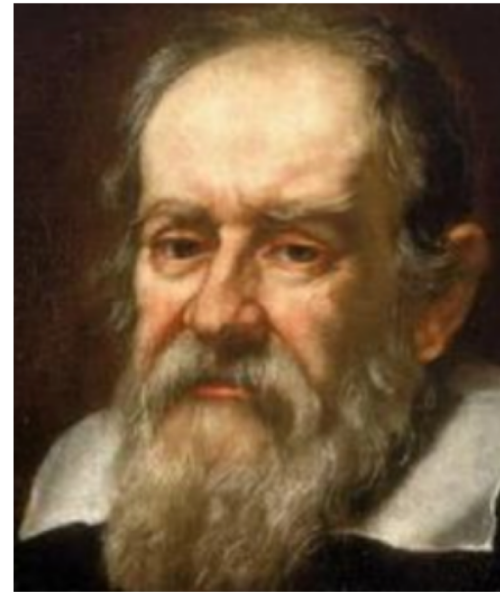
4. Concluding remarks and discussions

1. Clean Numerical Simulation (CNS) provides us a **new tool** and **benchmark solution** to study chaos and turbulence and to attack some **open questions**
2. Micro-level uncertainty might be the **origin** of some macroscopic randomness: the **whole world** is essentially **random**
3. A new concept **ultra-chaos** is proposed, which is a **high disorder** than normal-chaos
4. For an ultra-chaos, **all** numerical & experimental methods are **invalid**: a great **challenge** in science

4. Concluding remarks and discussions

- Modern science is based on **experiments**
- **Repeatability** of experiment is very important and necessary
- For an ultra-chaos, repeatability is **impossible** even in **statistics**
- How and what can we do for an **ultra-chaos**?

伽利略



比萨斜塔



modern science
= experiments + theory

4. Concluding remarks and discussions

CNS: a new tool for chaos and turbulence

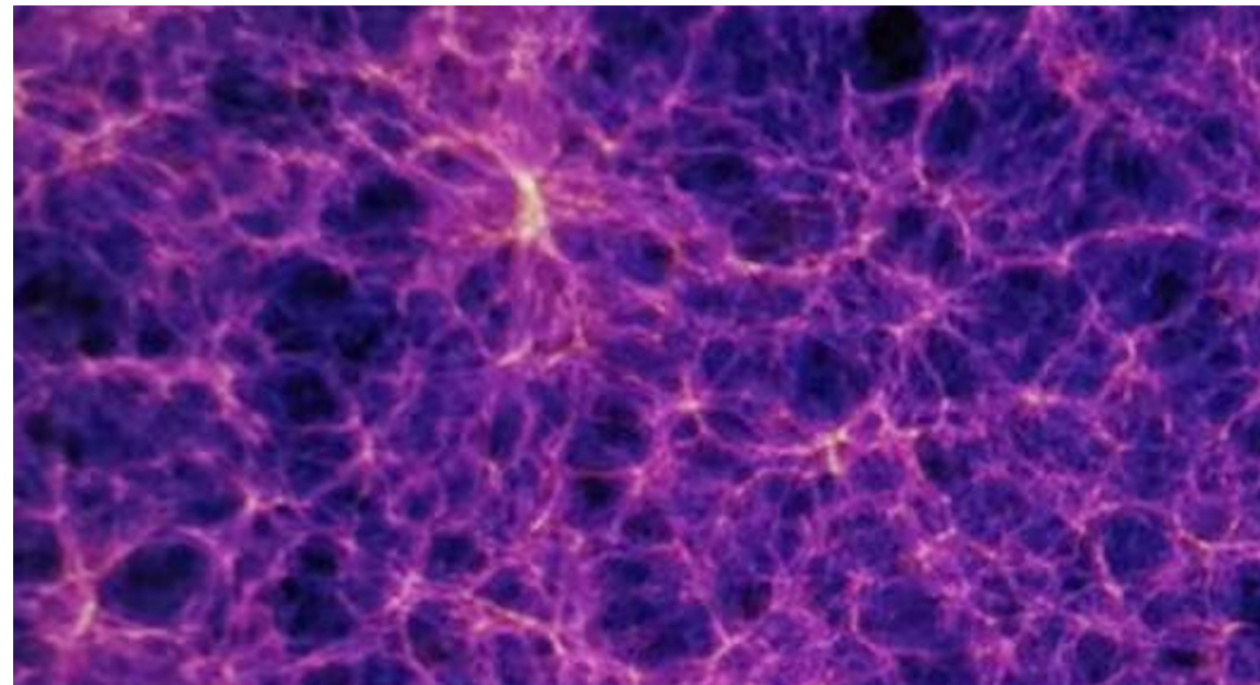
**A truly new method can always
bring something new and different!**

(A) Can we build a **data-base** of periodic orbits of three-body system so as to find a **non-hierarchical triple system** ?

(B) Can we apply the CNS to solve **N-body problem**?



马里亚纳
海沟生物
10900米



千禧年问题

Navier-Stokers 方程组：在适当的边界及初始条件下，对3维Navier-Stokers方程组证明（或反证）其光滑解的存在性。

Open Question

Landau-Lifschitz-Navier-Stokers 方程组：在适当的边界及初始条件下，对3维Landau-Lifschitz-Navier-Stokers方程组证明（或反证）其统计结果对微小扰动不敏感。

叔本华：生命的首要任务是“存在”，紧随其后的是“避开无聊”；满足就意味着无聊，好奇心正是我们挣脱出去的通行证。



超前的研究，大多数一开始都是无用的！

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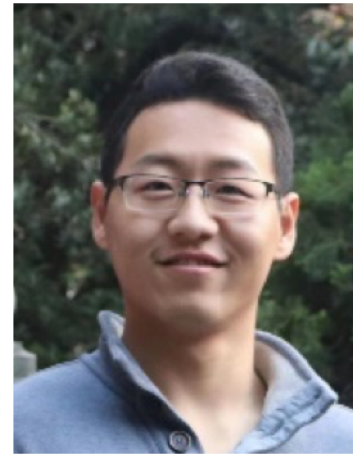
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