High-accuracy numerical integrator for general dynamical systems using vector-field decomposition and reccurence formula

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一般の力学系に対する
ベクトル場分割と漸化式を用いた高精度数値積分法

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Background and Motivation

- A numerical integration algorithm with arbitrarily high order has been developed for Hamiltonian systems, especially for a charged particle motion recently:
  [M. Furukawa, A. Matsuyama and Y. Ohkawa, Plasma Fusion Res. **11**, 1303003 (2016).]
  - Explicit method
  - Non-canonical variables are used
  - Poisson tensor is decomposed
  - Extended phase space is introduced for time-dependent EM fields
    - Note that the algorithm by exponential operator decomposition was developed for separable Hamiltonian in canonical variables
      [Masuo Suzuki, Phys. Lett. A (1990, 1992).]
      [Haruo Yoshida, Phys. Lett. A (1990).]

- The motivation of this study is to extend the algorithm to general dynamical systems
  - with odd number of degrees of freedom
  - of which vector field is compressible

Hamiltonian Mechanics of charged particle in time-dependent EM fields

[M. Furukawa, A. Matsuyama and Y. Ohkawa, Plasma Fusion Res. **11**, 1303003 (2016).]

- Let us consider motion of a charged particle in electric and magnetic fields

m : mass
e : charge
$\boldsymbol{q}$: canonical coordinate
$\boldsymbol{p}$: canonical momentum
$\phi(\boldsymbol{q}, t)$: electrostatic potential
$\boldsymbol{A}(\boldsymbol{q}, t)$: vector potential
$\mathcal{E}$: energy

- Hamiltonian is given by

$$\bar{H}[\boldsymbol{q}, \boldsymbol{p}, t] := \frac{(\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{q}, t))^2}{2m} + e\phi(\boldsymbol{q}, t)$$

- Let us introduce extended phase space, where

$$\bar{\boldsymbol{z}} := (\bar{\boldsymbol{q}}, \bar{\boldsymbol{p}})^{\mathrm{T}} = (q_1, q_2, q_3, t, p_1, p_2, p_3, -\mathcal{E})^{\mathrm{T}}$$

- Then the Hamilton's equation can be written as

$$\dot{\bar{\boldsymbol{z}}} = \bar{\mathcal{J}}\partial_{\bar{\boldsymbol{z}}}\bar{H} \quad \text{with} \quad \bar{\mathcal{J}} := \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix}$$

  - Dot denotes derivative with respect to "time" variable τ
  - 1st-3rd components are $\dot{\boldsymbol{q}} = \partial_{\boldsymbol{p}} H$ and $\dot{\boldsymbol{p}} = -\partial_{\boldsymbol{q}} H$
  - 4th componens are $\dot{t} = 1$ and $-\dot{\mathcal{E}} = -\partial_t H$

- If we write the vector field as

$$\partial_{\bar{\boldsymbol{z}}}\bar{H} := V_H[\bar{\boldsymbol{z}}]$$

the formal solution is

$$\bar{\boldsymbol{z}}(\tau) = \mathrm{e}^{\tau V_H}\bar{\boldsymbol{z}}(0)$$

Exponential operator decomposition

[M. Furukawa, A. Matsuyama and Y. Ohkawa, Plasma Fusion Res. **11**, 1303003 (2016).]

- Since the Hamiltonian is not separable for the canonical variables
- Let us introduce non-canonical variables:

$$\bar{\boldsymbol{z}}' := (x, y, z, t, v_x, v_y, v_z, -\mathcal{E})^{\mathrm{T}}$$

Then the Hamiltonian becomes

$$\bar{H}'(\bar{\boldsymbol{x}}, \bar{\boldsymbol{v}}) = \frac{m}{2}\boldsymbol{v}^2 + e\phi(\boldsymbol{x}, t) - \mathcal{E}$$

- The evolution equation becomes

$$\dot{\bar{\boldsymbol{z}}}' = \bar{\mathcal{J}}'\partial_{\bar{\boldsymbol{z}}'}\bar{H}'(\bar{\boldsymbol{z}}') \quad \text{with} \quad \bar{\mathcal{J}}' = \frac{1}{m}\left(\begin{array}{c|c|ccc|c} 0 & \mathbf{0} & & 1 & & \mathbf{0} \\ \hline \mathbf{0}^{\mathrm{T}} & 0 & & \mathbf{0}^{\mathrm{T}} & & 1 \\ \hline & & 0 & \frac{e}{m}B_z & -\frac{e}{m}B_y & \\ -1 & \mathbf{0} & -\frac{e}{m}B_z & 0 & \frac{e}{m}B_x & -e\partial_t\boldsymbol{A} \\ & & \frac{e}{m}B_y & -\frac{e}{m}B_x & 0 & \\ \hline \mathbf{0}^{\mathrm{T}} & -1 & & e\partial_t\boldsymbol{A}^{\mathrm{T}} & & 0 \end{array}\right)$$

- We decompose the Poisson tensor as

$$\bar{\mathcal{J}}' = \sum_{\alpha=1}^{8}\bar{\mathcal{J}}'_\alpha \quad \text{with} \quad \bar{\mathcal{J}}'_1 := \frac{1}{m}\begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad \text{for } \alpha = 1 \text{ and so on}$$

- Then the vector field is decomposed as

$$V_H[\bar{\boldsymbol{z}}'] = \sum_{\alpha=1}^{8} V_\alpha[\bar{\boldsymbol{z}}'] \quad \text{with} \quad V_\alpha[\bar{\boldsymbol{z}}'] := \bar{\mathcal{J}}'_\alpha\partial_{\bar{\boldsymbol{z}}'}\bar{H}(\bar{\boldsymbol{z}}')$$

Exponential operator decomposition (cont'd)

[M. Furukawa, A. Matsuyama and Y. Ohkawa, Plasma Fusion Res. **11**, 1303003 (2016).]

- The formal solution is written by exponential operator expressing the time advancement:

$$\bar{\boldsymbol{z}}'(\tau) = \mathrm{e}^{\tau \sum_{\alpha=1}^{8} \bar{V}'_\alpha [\bar{\boldsymbol{z}}']} \bar{\boldsymbol{z}}'(0)$$

- The exponential operator can be approximated as

$$\mathrm{e}^{\tau \sum_{\alpha=1}^{8} \bar{V}'_\alpha} = \Pi_{\alpha=1}^{8} \mathrm{e}^{\tau \bar{V}'_\alpha} + \mathcal{O}(\tau^2)$$

  - The right hand side (omitting the $\mathcal{O}(\tau^2)$ terms) means sequential operations of $\mathrm{e}^{\tau \bar{V}'_\alpha}$
  - Each of the decomposed exponential operators can be calculated exactly

- This approximation can be used as a 1st-order algorithm for small time interval $\Delta\tau$
  - We call this algorithm as $G_1(\tau)$

- The 2nd-order algorithm ($S_2(\tau)$) can be constructed by time-symmetric decomposition

$$S_2(\tau) = \mathrm{e}^{\frac{1}{2}\tau \bar{V}'_1} \mathrm{e}^{\frac{1}{2}\tau \bar{V}'_2} \mathrm{e}^{\frac{1}{2}\tau \bar{V}'_3} \mathrm{e}^{\frac{1}{2}\tau \bar{V}'_4} \mathrm{e}^{\frac{1}{2}\tau \bar{V}'_5} \mathrm{e}^{\frac{1}{2}\tau \bar{V}'_6} \mathrm{e}^{\frac{1}{2}\tau \bar{V}'_7} \mathrm{e}^{\tau \bar{V}'_8} \mathrm{e}^{\frac{1}{2}\tau \bar{V}'_7} \mathrm{e}^{\frac{1}{2}\tau \bar{V}'_6} \mathrm{e}^{\frac{1}{2}\tau \bar{V}'_5} \mathrm{e}^{\frac{1}{2}\tau \bar{V}'_4} \mathrm{e}^{\frac{1}{2}\tau \bar{V}'_3} \mathrm{e}^{\frac{1}{2}\tau \bar{V}'_2} \mathrm{e}^{\frac{1}{2}\tau \bar{V}'_1}$$

- By combining several steps of $S_{2(m-1)}(\tau)$ nicely, we can construct $S_{2m}(\tau)$

Extension for general vector fields

- The arbitrarily high order of accuracy is achieved because
  - time advancement by each exponential operator is performed exactly
  - truncation error only arises when we decompose the full exponential operator

- If we can decompose the vector field of a general dynamical system, where each of the decomposed exponential operator can be integrated exactly, we may obtain a numerical integration algorithm with arbitrarily high order as in the case of the charged particle motion

- Two examples are shown in this presentation

Case 1 Damped oscillator

The vector field is compressible, but the dynamics is regular (no chaos)

Case 2 Lorenz model

The vector field is compressible
The dimension of the phase space is three (odd)
The dynamics can be chaotic

Case 1

Damped oscillator : formulation

- The governing equations are

$$\dot{\boldsymbol{z}} = \boldsymbol{V}[\boldsymbol{z}] \qquad \text{with} \qquad \dot{\boldsymbol{z}} := \begin{pmatrix} x \\ v \end{pmatrix} \qquad \text{and} \qquad \boldsymbol{V} := \begin{pmatrix} v \\ -x - \nu v \end{pmatrix}$$

- The formal solution is

$$\boldsymbol{z}(t) = \mathrm{e}^{t\boldsymbol{V}} \boldsymbol{z}(0)$$

- Let us decompose the vector field as

$$\boldsymbol{V} = \boldsymbol{V}_x + \boldsymbol{V}_v \qquad \text{with} \qquad \boldsymbol{V}_x := \begin{pmatrix} v \\ 0 \end{pmatrix} \qquad \text{and} \qquad \boldsymbol{V}_v := \begin{pmatrix} 0 \\ -x - \nu v \end{pmatrix}$$

- Then the 1st-order approximation of the exponential operator becomes

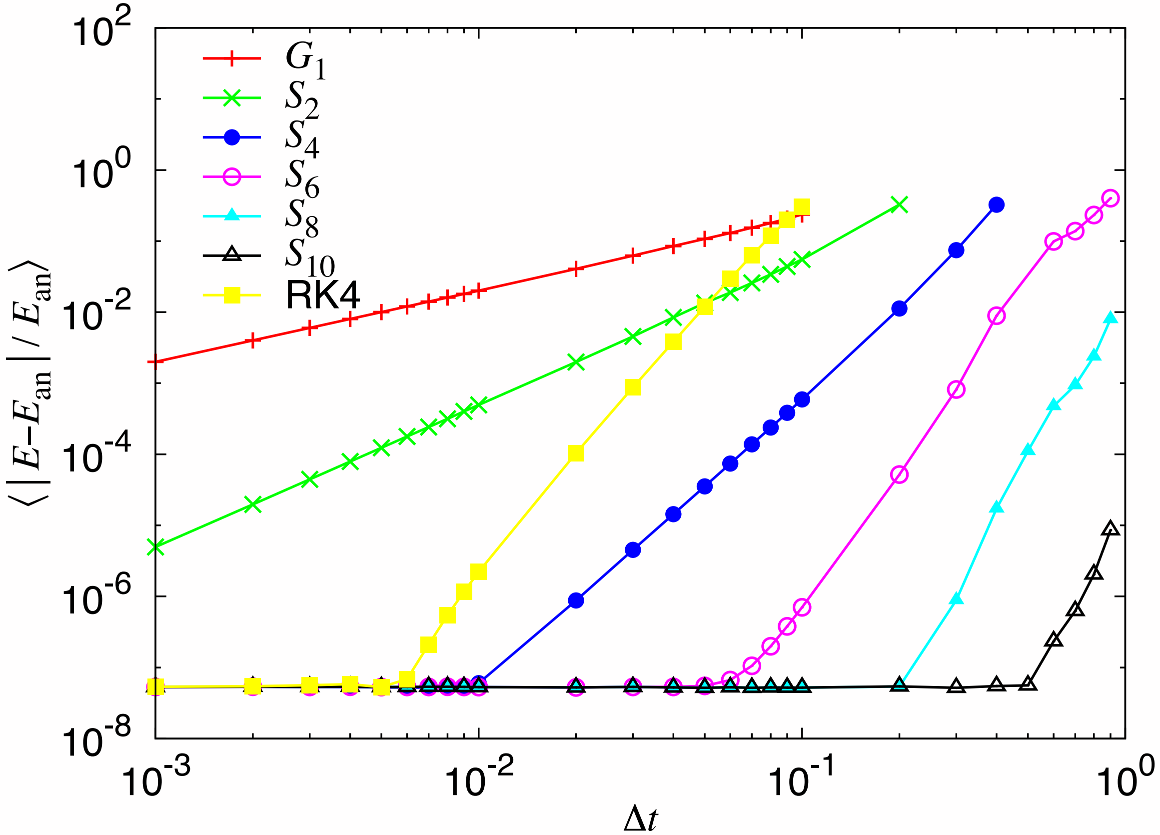
$$\mathrm{e}^{t\boldsymbol{V}} = \mathrm{e}^{t\boldsymbol{V}_x} \mathrm{e}^{t\boldsymbol{V}_v} + \mathcal{O}(t^2)$$

- Each operation of the decomposed exponential operators can be calculated exactly as
  - $\mathrm{e}^{t\boldsymbol{V}_x}: \quad x(t) = x(0) + v(0)t$
  - $\mathrm{e}^{t\boldsymbol{V}_v}: \quad v(t) = -\frac{1}{\nu}x(0) + \mathrm{e}^{t\nu}\left(\frac{1}{\nu}x(0) + v(0)\right)$
- Higher-order algorithms can be constructed by imposing the time-reversal symmetry (2nd order) and the recurrence formula (arbitrarily high order)

Damped oscillator : numerical results

- The accuracy of the numerical results is evaluated by comparison of the energy with analytic solution:

$$\left\langle \frac{|E - E_{\rm an}|}{E_{\rm an}} \right\rangle := \frac{1}{T} \int_0^T \mathrm{d}t \, \frac{|E - E_{\rm an}|}{E_{\rm an}}$$



- The theoretical order of accuracy is almost achieved ($(\Delta t)^8$ for S_{10})

Case 2

Lorenz model : formulation

- The Lorenz model is given by

$$\dot{\boldsymbol{z}} = \boldsymbol{V}[\boldsymbol{z}] \quad \text{with} \quad \boldsymbol{z} := \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} \quad \text{and} \quad \boldsymbol{V}[\boldsymbol{z}] := \begin{pmatrix} -\sigma X + \sigma Y \\ rX - Y - XZ \\ -bZ + XY \end{pmatrix}$$

- The vector field is decomposed as

$$\boldsymbol{V} = \boldsymbol{V}_X + \boldsymbol{V}_Y + \boldsymbol{V}_Z$$

$$\boldsymbol{V}_X := \begin{pmatrix} -\sigma X + \sigma Y \\ 0 \\ 0 \end{pmatrix} \qquad \boldsymbol{V}_Y := \begin{pmatrix} 0 \\ rX - Y - XZ \\ 0 \end{pmatrix} \qquad \boldsymbol{V}_Z := \begin{pmatrix} 0 \\ 0 \\ -bZ + XY \end{pmatrix}$$

- Then the 1st-order approximation of the exponential operator becomes

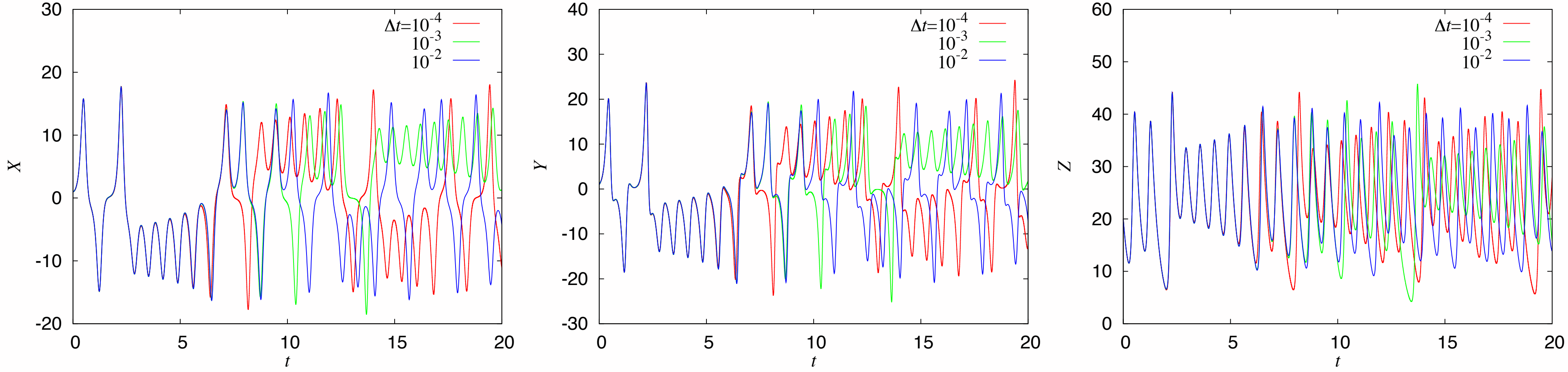
$$\mathrm{e}^{t\boldsymbol{V}} = \mathrm{e}^{t\boldsymbol{V}_X}\mathrm{e}^{t\boldsymbol{V}_Y}\mathrm{e}^{t\boldsymbol{V}_Z} + \mathcal{O}(t^2)$$

- Each operation of the decomposed exponential operators can be calculated exactly as
  - $\mathrm{e}^{t\boldsymbol{V}_X}$: $X(t) = Y(0) + \mathrm{e}^{-t\sigma}(X(0) - Y(0))$
  - $\mathrm{e}^{t\boldsymbol{V}_Y}$: $Y(t) = rX(0) - X(0)Z(0) + \mathrm{e}^{-t}(Y(0) - rX(0) + X(0)Z(0))$
  - $\mathrm{e}^{t\boldsymbol{V}_Z}$: $Z(t) = \frac{1}{b}X(0)Y(0) + \mathrm{e}^{-tb}\left(Z(0) - \frac{1}{b}X(0)Y(0)\right)$
- Higher-order algorithms are similarly constructed

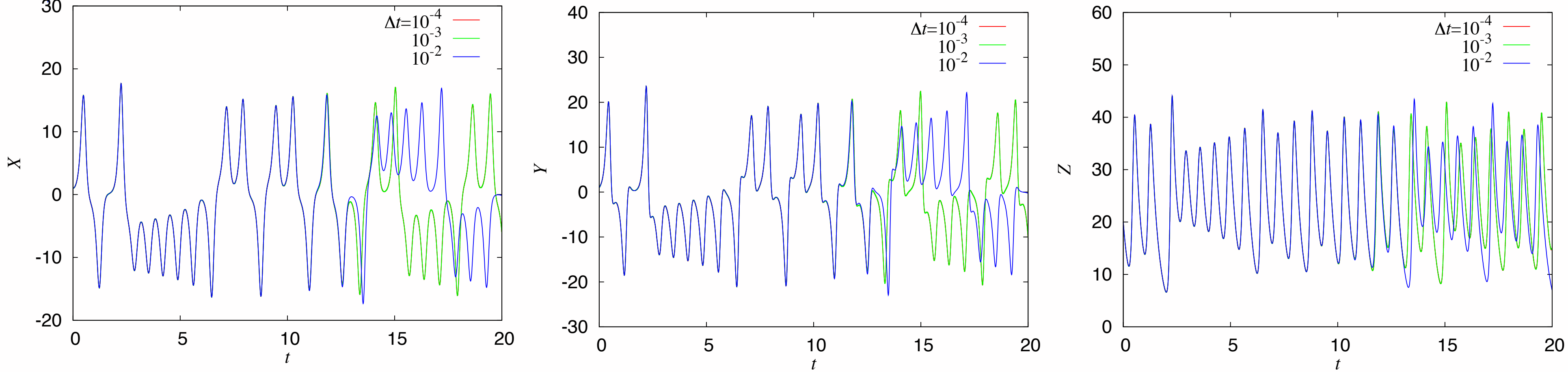
Case 2 Lorenz model : numerical results (convergence)

- Parameters: $\sigma = 10$, $b = \dfrac{8}{3}$, $r = 28$, $X(0) = 1$, $Y(0) = 1$, $Z(0) = 20$

- $S_4(\Delta t)$



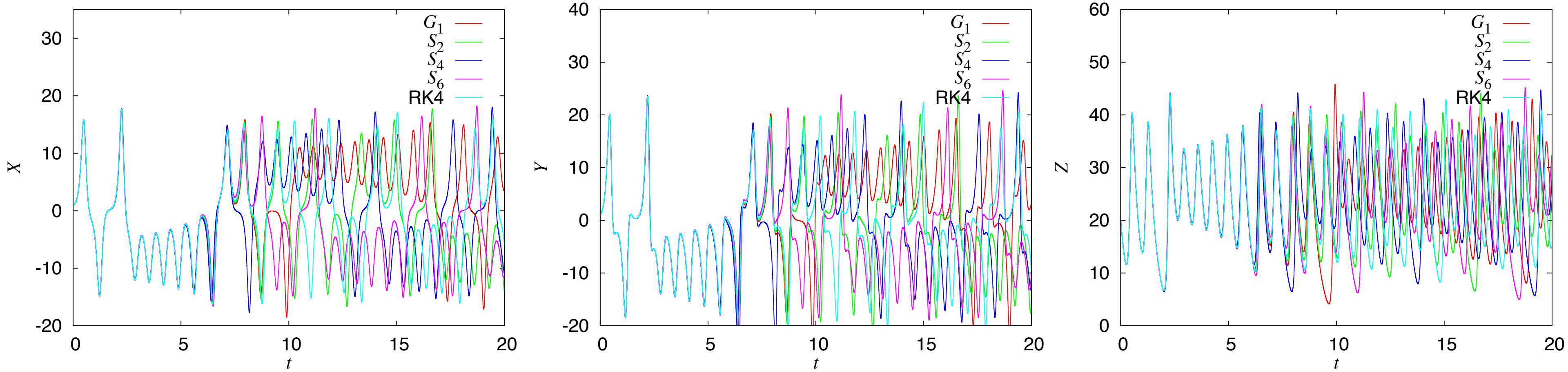
- RK4



- RK4 seems to show better convergence property

Case 2 Lorenz model : numerical results (convergence) : cont'd

- Parameters: $\sigma = 10$, $b = \dfrac{8}{3}$, $r = 28$, $X(0) = 1$, $Y(0) = 1$, $Z(0) = 20$
- $\Delta t = 10^{-4}$

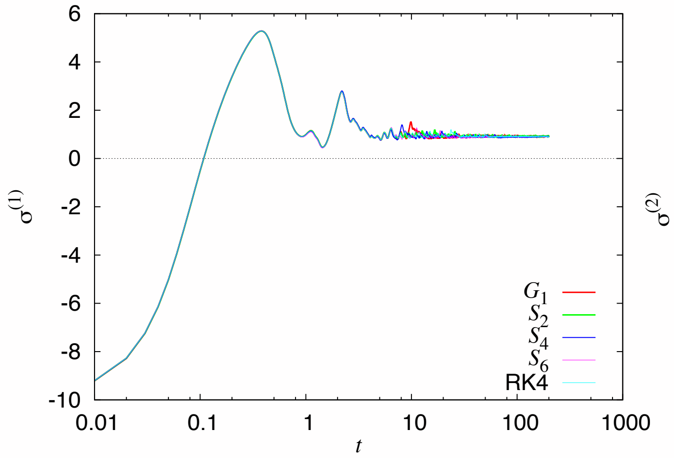


- The numerical results by various algorithms start to deviate around $t \simeq 7$

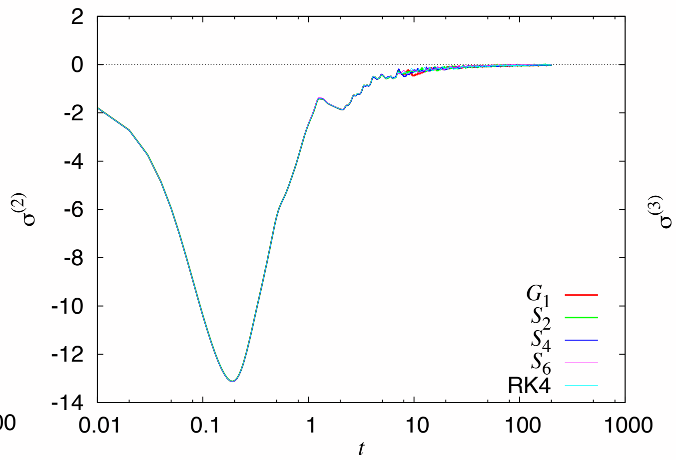
Case 2 Lorenz model : numerical results (Liapunov exponent)

- Parameters: $\sigma = 10$, $b = \frac{8}{3}$, $r = 28$, $X(0) = 1$, $Y(0) = 1$, $Z(0) = 20$

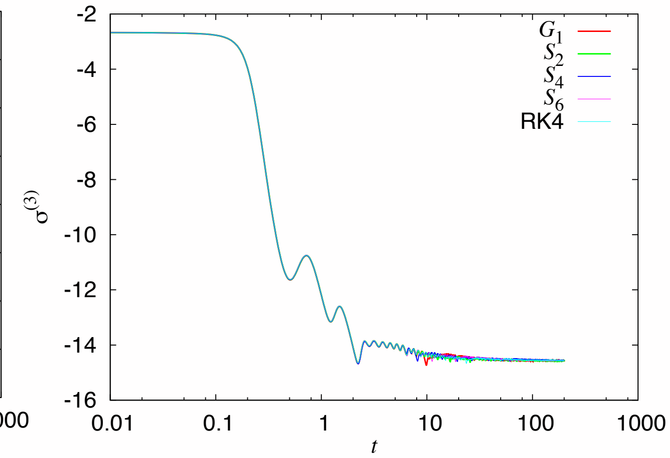
$\sigma^{(1)} \simeq 0.90$



$\sigma^{(2)} \simeq -1.4 \times 10^{-2}$



$\sigma^{(3)} \simeq -15$



- Since $e^{0.9\times7} \simeq 5 \times 10^2$, an error of $\mathcal{O}(10^{-3})$ is amplified to $\mathcal{O}(1)$ during $t = 0$ to $t \simeq 7$

- We have not clarified the reason yet

- Note that numerical results with parameters without chaos well agreed among algorithms

Conclusions

- The numerical integration algorithm with arbitrarily high order has been extended to general dynamical systems
  - odd number of degrees of freedom
  - compressible vector field
  - although more testing is needed
- Numerical results for the damped oscillator showed good convergence property
- Convergence property for the Lorenz model (parameters giving chaos) was better for the 4th-order Runge-Kutta method
  - We have not clarified the reason yet
  - Note that the numerical results without chaos well agreed among algorithms