Structure-Preserving Exponential Integrators

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Acknowledgements

Joint work with

- Constance Schober, Professor UCF
- Laura Norena, UCF student, currently with Valencia College
- Dwayne Floyd, UCF student, currently with DOD
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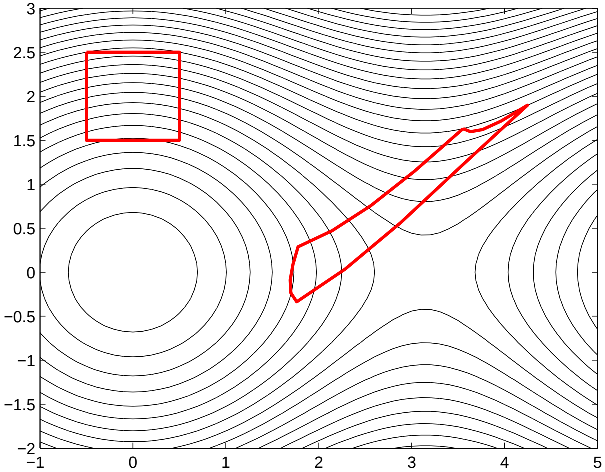
- NTNU Department of Mathematical Sciences for office space, facilities, and a stimulating research environment

Background: Phase space area

Example: Phase portrait for the pendulum problem, $\ddot{q} + \sin(q) = 0$



Background: Simple conservative systems

Models from Newtons 2nd law: $\ddot{q} + \nabla_q V(q) = 0$

- The energy $H = \frac{1}{2}\dot{q}^2 + V(q)$ is an invariant.

$$\frac{d}{dt}H = \frac{d}{dt}\left(\frac{1}{2}\dot{q}^2 + V(q)\right) = \dot{q}\left(\ddot{q} + \nabla_q V(q)\right) = 0$$

- The symplectic form $\omega = dq \wedge d\dot{q}$ is invariant.
  The variational equation $d\ddot{q} + V_{qq}(q)dq = 0$ implies

$$0 = dq \wedge d\ddot{q} + dq \wedge V_{qq}(q)dq = \frac{d}{dt}\left(dq \wedge d\dot{q}\right)$$

  because V_{qq} symmetric implies $dq \wedge V_{qq}(q)dq = 0$.
  $\frac{d}{dt}\omega = 0$ corresponds to conservation of phase space area.

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- Unfortunately, it is not possible, in general, to preserve both energy and the symplectic form at the same time.
- Symplecticity is not a physical property, so many practitioners prefer energy-preserving methods.
- One benefit of preserving symplecticity is that energy is nearly preserved.

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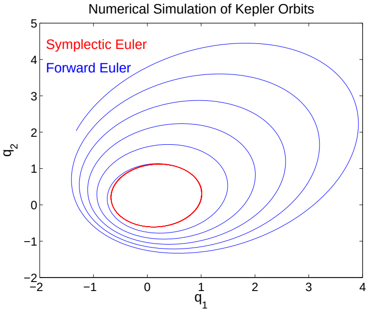
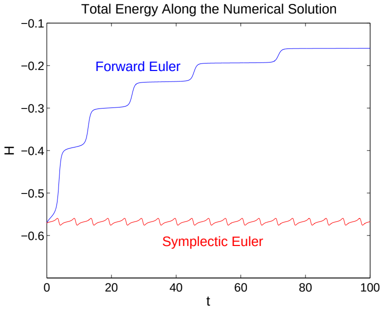
Numerical solutions:
One method is conservative the other is non-conservative

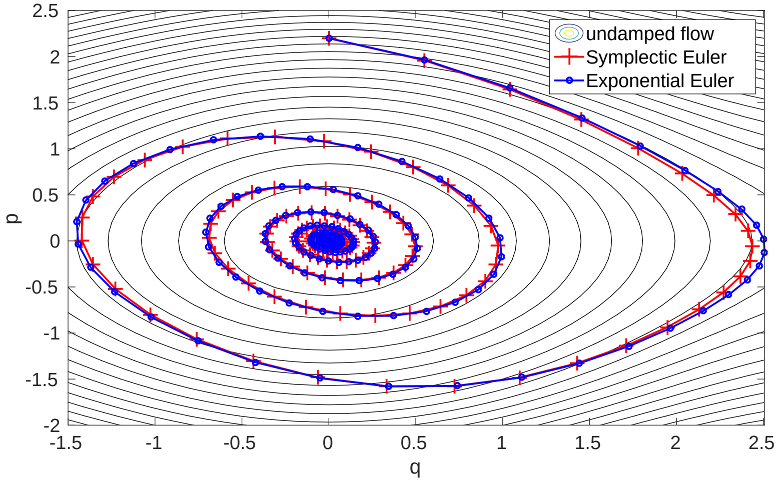




Background: Books on structure-preserving algorithms

- R.E. Mickens, *Nonstandard Finite Difference Models of Differential Equations*, 1993
- J.M. Sanz-Serna and M.P. Calvo, *Numerical Hamiltonian Problems*, 1994
- A. Stuart and A.R. Humphries, *Dynamical Systems and Numerical Analysis*, 1998
- E. Hairer, G. Wanner, and C. Lubich, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*, 2002
- B. Leimkuhler and S. Reich, *Simulating Hamiltonian Dynamics*, 2005
- D. Furihata and T. Matsuo, *Discrete Variational Derivative Method: A Structure-Preserving Numerical Method for Partial Differential Equations*, 2010
- X. Wu, X. You, and B. Wang, *Structure-Preserving Algorithms for Oscillatory Differential Equations*, 2013

Trajectories for a damped pendulum problem, $\ddot{q} + \gamma\dot{q} + \sin(q) = 0$



Background: Conformal Symplectic Models and Methods

- McLachlan and Perlmutter (2001): conformal Hamiltonian systems; contraction of the symplectic form

$$\partial_t \omega = -2\gamma\omega \qquad \Longleftrightarrow \qquad \omega(t) = e^{-2\gamma t}\omega(0)$$

- McLachlan and Quispel (2001) and (2002): splitting methods that preserve conformal symplecticity; they satisfy

$$\omega^{n+1} = e^{-2\gamma h}\omega^n$$

where $h = t_{n+1} - t_n$ is the step size.

Splitting Methods for solving $\dot{y} = N(y) - \gamma y$

1. Solve $\dot{y} = N(y)$ with a conservative (symplectic) method
2. Solve $\dot{y} = -\gamma y$ exactly: $y(t) = y_0 e^{-\gamma t}$
3. Compose the flow maps to get a conformal symplectic scheme

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Generalizations

Consider the IVP

$$\dot{y}(t) = N(y(t)) - \gamma(t)y(t), \quad y(0) = y_0$$

where $y \in \mathbb{R}^d$ with $d \in \mathbb{N}$, $\gamma : \mathbb{R} \to \mathbb{R}$, and $N : \mathbb{R}^d \to \mathbb{R}^d$

Definition of conformal invariant

$\mathcal{I} : \mathbb{R}^d \to \mathbb{R}$ is a *conformal invariant* for the IVP if $\frac{d}{dt}\mathcal{I} = -\gamma(t)\mathcal{I}$.

Note: $\mathcal{I}(y(t)) = e^{-\int_0^t \gamma(s)ds}\mathcal{I}(y_0) \implies \frac{d}{dt}\mathcal{I} = -\gamma(t)\mathcal{I}$.

Definition of numerical preservation

A numerical method *preserves* a conformal invariant if it satisfies

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Examples of conformal invariants

- Pendulum: $\ddot{q} + 2\gamma\dot{q} + \sin q = 0$
  $\mathcal{I} = dq \wedge d\dot{q}$
- Oscillator: $\ddot{q} + 2\gamma\dot{q} + \kappa^2 q = 0$
  $\mathcal{I} = (\kappa^2 q^2 + \dot{q}^2)/2 + \gamma q\dot{q}$
- Rigid Body: $\dot{y} = B(y)\nabla H(y) - \gamma y$ with $y = [y_1, y_2, y_3]^T$
  $\mathcal{I} = y_1^2 + y_2^2 + y_3^2$ and $H(y) = \frac{1}{2}\left(\frac{y_1^2}{I_1} + \frac{y_2^2}{I_2} + \frac{y_3^2}{I_3}\right)$
- Klein-Gordon: $u_{tt} - u_{xx} + cu + 2\gamma u_t = 0$
  $\mathcal{I} = \int u_t u_x \; dx$
- Schrödinger: $\mathtt{i}\psi_t + \psi_{xx} + V'(|\psi|^2)\psi + \mathtt{i}\gamma\psi = 0$
  $\mathcal{I} = \int |\psi|^2 \; dx$
- Camassa Holm: $u_t - u_{xxt} + 3uu_x + \gamma(u - u_{xx}) = 2u_x u_{xx} + uu_{xxx}$
  $\mathcal{I} = \int (u^2 + u_x^2) \; dx$
- KdV: $u_t + uu_x + u_{xxx} + 2\gamma u = 0$
  $\mathcal{I} = \int u \; dx$

Exponential Runge-Kutta Methods

Runge-Kutta type methods for solving $\dot{y} = N(y) - \gamma y$

$$Y_i = \phi_i(h;\gamma_n) y_n + h \sum_{j=1}^{s} a_{ij}(h;\gamma_n) N(Y_j), \quad i = 1, \ldots, s,$$

$$y_{n+1} = \phi_0(h;\gamma_n) y_n + h \sum_{i=1}^{s} b_i(h;\gamma_n) N(Y_i).$$

The *coefficient functions*, ϕ_i, ϕ_0, a_{ij}, and b_i satisfy

$$\phi_i(h;0) = \phi_0(h;0) = 1, \qquad a_{ij}(h;0) = \alpha_{ij}, \qquad b_i(h;0) = \beta_i$$

for all $i, j = 1, 2, \ldots, s$.

Similar results hold for partitioned exponential RK methods.

Numerical structure preservation

Theorem (Bhatt & M, *SIAM J. Sci. Comp.* 2017)

An ERK method is conformal symplectic and preserves conformal quadratic invariants if it has scalar coefficient functions which satisfy $\phi_0 = e^{-\int_{t_n}^{t_{n+1}} \gamma(s)ds}$ *and*

$$a_{ji} b_i \frac{\phi_0}{\phi_i} + a_{ij} b_j \frac{\phi_0}{\phi_j} - b_i b_j = 0 \qquad \forall i, j = 1, 2, \ldots, s.$$

Example

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Example

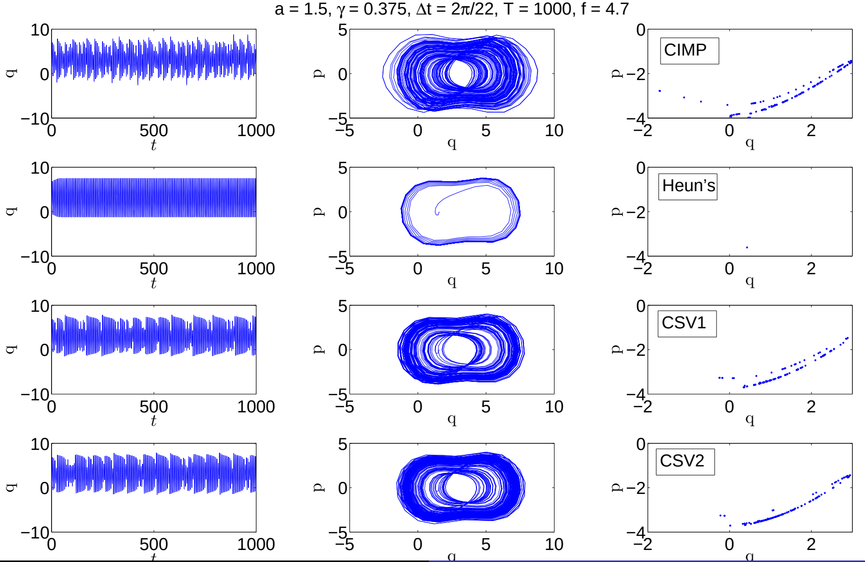
Setting $s = 1$, $a_{11} = 1/2$, $b_1 = e^{-\int_{t_{n+1/2}}^{t_{n+1}} \gamma(s) ds}$, $\phi_1 = e^{-\int_{t_n}^{t_{n+1/2}} \gamma(s) ds}$, gives an implicit midpoint type method

$$w_1 y_{n+1} - w_0 y_n = hN \left(\frac{1}{2} (w_1 y_{n+1} + w_0 y_n) \right),$$

with $w_0 = \phi_1$ and $w_1 = 1/b_1$.

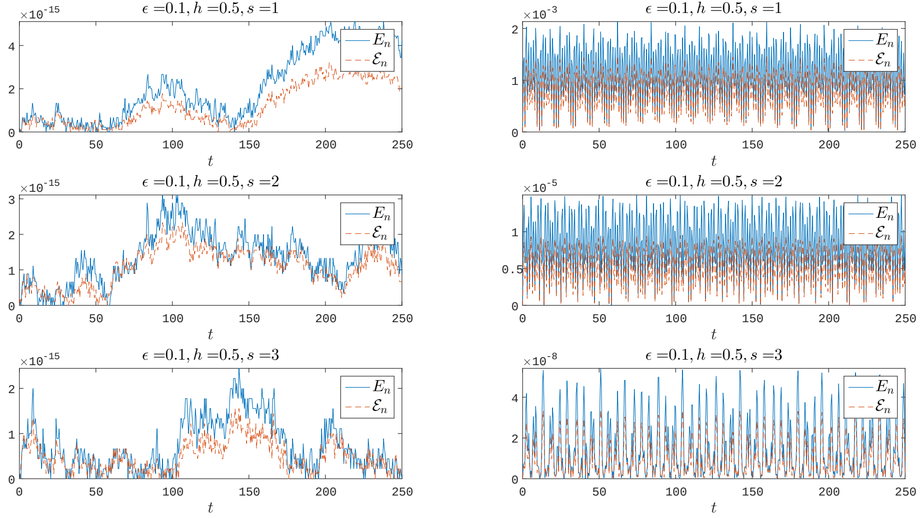
Forced-Damped Chaotic Pendulum

$$\dot{q} = p, \qquad \dot{p} = -a^2 \sin(q) + f_d \sin(t) - 2\gamma p$$



Periodically perturbed rigid body, $\gamma(t) = \epsilon\cos(2t)$

Conformal invariant error. Left: ERK; Right: Gauss-Legendre



Damped-Driven NLS

DDNLS1: $i\psi_t + \psi_{xx} + i\gamma\psi + (\alpha + i\beta)\psi + V'(|\psi|)\psi = 0$

Case $\alpha = c\cos(\omega t)$ and $\beta = c\sin(\omega t)$ studied by X. Chen and R. Wei (1994), Jie-Hua et al. (2002), W. Hu et al. (2017)

Norm Conservation with $\psi = p + iq$ and $\theta(t) = \int_0^t (\gamma + \beta(s))ds$

$$\partial_t(e^{2\theta(t)}(p^2 + q^2)) + \partial_x(2e^{2\theta(t)}(pq_x - qp_x)) = 0,$$

DDNLS2: $i\psi_t + \psi_{xx} + i\gamma\psi + (\alpha + i\beta)\psi^* + V'(|\psi|)\psi = 0$

Case $\alpha = c\cos(\omega t)$ and $\beta = c\sin(\omega t)$ studied extensively by I.V. Barashenkov and co-authors

Momentum Conservation with $\psi = p + iq$

$$0 = \partial_t\left(e^{2\gamma t}(pq_x - qp_x)\right) + \partial_x\left(e^{2\gamma t}\left(p_x^2 + q_x^2 - pq_t + qp_t - \alpha(q^2 - p^2) + 2\beta qp + V(p^2 + q^2)\right)\right)$$

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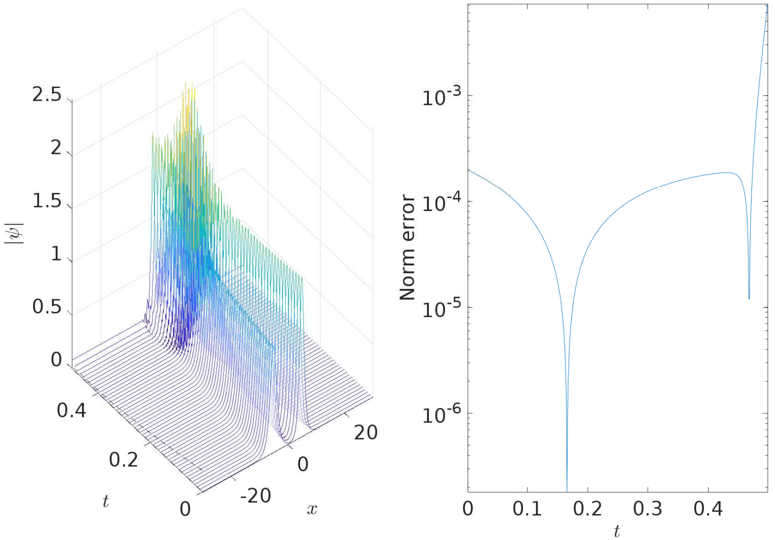
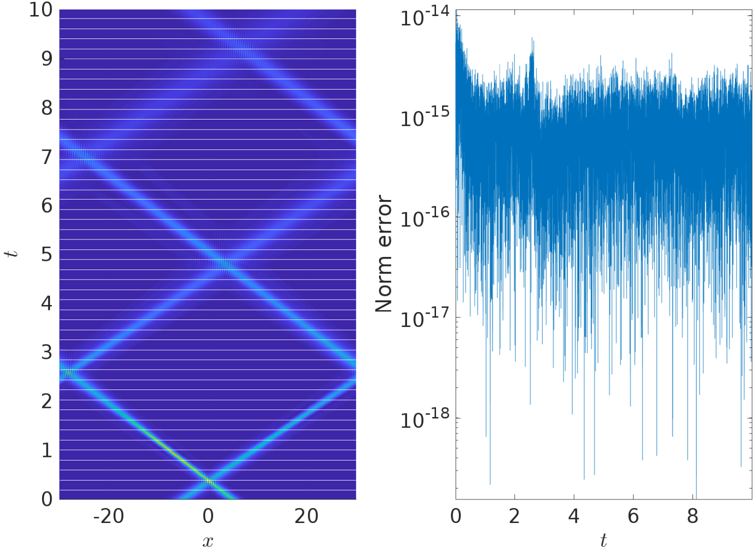
Soliton collision: GL method with $c = 0.2$, $\gamma = 0.1$, $\omega = \pi$



Soliton collision: Exp method w/ $c = 0.2$, $\gamma = 0.1$, $\omega = \pi$



Discrete Gradient Methods

Consider $\dot{y} = B(y)\nabla H(y) - \gamma(t)y$. If $C(y)$ is a quadratic Casimir in the case $\gamma = 0$, then the system satisfies

$$\frac{d}{dt}C(y(t)) = -2\gamma(t)C(y(t)) \quad \Longleftrightarrow \quad C(y(t)) = e^{-2\int_0^t \gamma(s)ds} C(y(0)).$$

The exponential discrete gradient method

$$\frac{e^{x_1}y_1 - e^{x_0}y_0}{h} = B\left(\frac{e^{x_1}y_1 + e^{x_0}y_0}{2}\right)\overline{\nabla}H\left(e^{x_0}y_0, e^{x_1}y_1\right)$$

with $x_\alpha := \int_{t_{n+1/2}}^{t_{n+\alpha}} \gamma(s)ds$ and

$$H(y_1)-H(y_0) = \overline{\nabla}H(y_0,y_1)(y_1-y_0), \qquad \lim_{y_1\to y_0} \overline{\nabla}H(y_0,y_1) = \nabla H(y_0)$$

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Energy Dissipation

For $\dot{y} = B(y)\nabla H(y) - \gamma(t)y$, energy is drained out according to

$$\frac{d}{dt}H = \nabla H(y)^T B(y)\nabla H(y) - \gamma\nabla H(y)^T y = -\gamma\nabla H(y)^T y,$$

Standard discrete gradient method satisfies

$$\frac{H(y_1) - H(y_0)}{h} = -\gamma_{1/2}\nabla H\left(y_{1/2}\right)^T y_{1/2} + \mathcal{O}(h^2).$$

Exponential discrete gradient method satisfies

$$\frac{H(y_1) - H(y_0)}{h} = -\gamma_{1/2}\frac{1}{2}\left(\nabla H(y_1)^T y_1 + \nabla H(y_0)^T y_0\right) + \mathcal{O}(\gamma_{1/2}^2 h^2),$$

Extensions to PDEs

We have seen ODEs that satisfy properties of the form

$$\frac{d}{dt}\mathcal{I} = -\gamma\mathcal{I}.$$

There are PDEs that satisfy properties of the form

$$P_t + Q_x = -aP - bQ.$$

which is a direct result of

$$\partial_t \left(e^{(at+bx)} P \right) + \partial_x \left(e^{(at+bx)} Q \right) = 0.$$

Thus, we say a numerical method preserves this property if it satisfies a discrete version of the property.

Examples

- Generalized Diffusionless Burgers-Fisher Equation

$$u_t + \beta u^\alpha u_x = \gamma u(1 - u^\alpha)$$

- Damped Linear KdV-Burgers Equation

$$u_t + u_{xxx} + \alpha u_{xx} + \beta u_x + \gamma u = 0$$

- Non-linear Schrödinger Type Equation

$$i\psi_t + \psi_{xx} + (\alpha + i\beta)\psi_x + (\delta + i\gamma)\psi + V'(|\psi|)\psi = 0$$

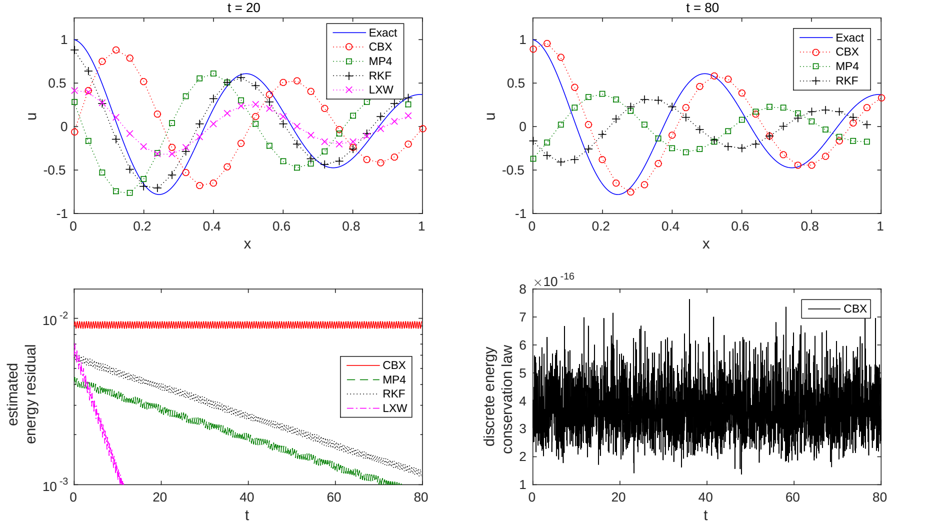
- Non-linear Wave Equation

$$u_{tt} + 2au_t - (\partial_x + 2b)\sigma'(u_x) + f'(u) = 0$$

- etc.

$u = e^{-x}\cos(4\pi(x - t))$ as solution of $u_t + u_x + u = 0$

$\Delta t = 0.025,\ \Delta x = 0.04$



Conclusion and Future Work

Summary

- General approach for constructing high order (Runge-Kutta-like) structure-preserving algorithms.
- The methods are designed for conservative equations that are perturbed by linear non-conservative terms.
- Various properties (relating to energy, momentum, mass, symplecticity, etc.) may be preserved.
- Dissipation rates are exactly preserved for linear problems.

Future Work

- Backward error analysis.
- Usefulness for spatial discretizations of PDEs.
- Extensions to problems where γ is a matrix.
- Construction of exponential time-differencing methods.

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