Geometric numerical integration

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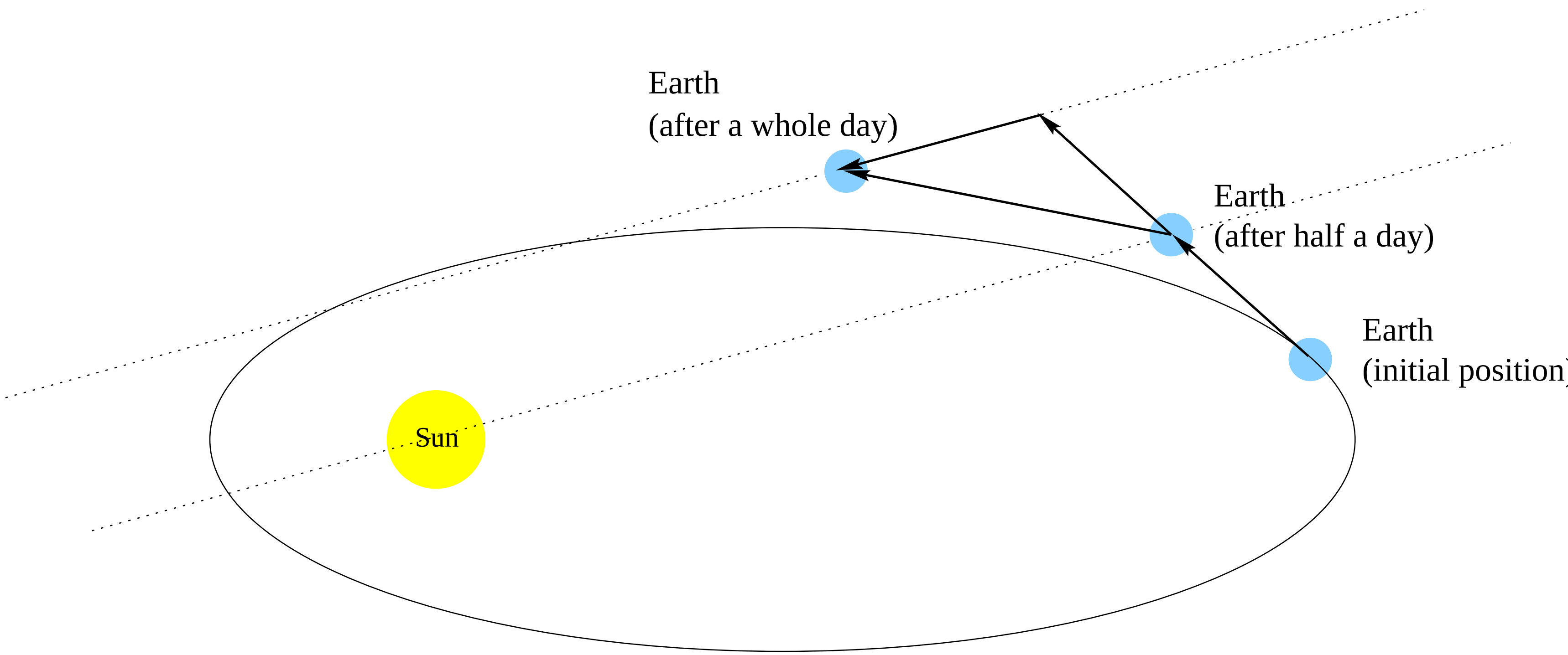
- A numerical method for a differential equation which inherits some property of the equation exactly.
- The property should be possible to impose exactly, while still constraining the solution in some useful way.
- Examples: preserving first integrals, symmetries, phase space volume, symplecticity for Hamiltonian systems, reversibility, Lyapunov functions

A basic example



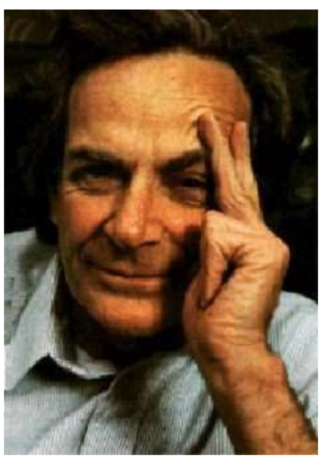
The leapfrog method

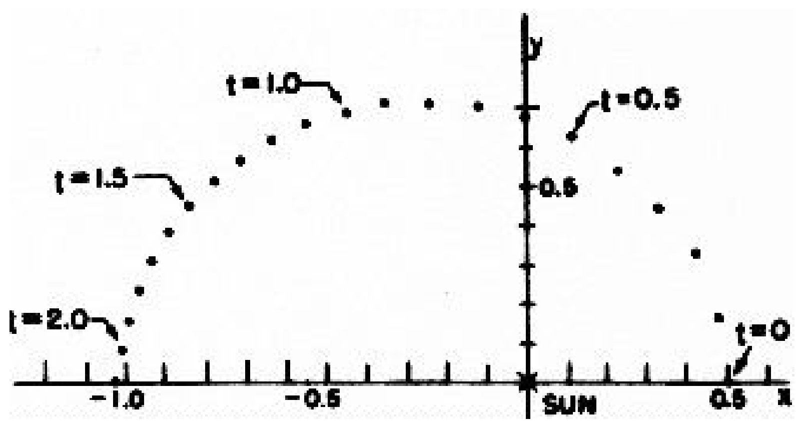
Loup Verlet, 1967

Feynman's *Lectures on Physics*

should use the acceleration midway between the two times at which the velocity is to be found. Thus the equations that we shall actually use will be something like this: the position later is equal to the position before plus ϵ times the velocity *at the time in the middle of the interval*. Similarly, the velocity at this halfway point is the velocity at a time ϵ before (which is in the middle of the previous interval) plus ϵ times the acceleration at the time t. That is, we use the equations

$$\begin{aligned} x(t+\epsilon) &= x(t) + \epsilon v(t+\epsilon/2), \\ v(t+\epsilon/2) &= v(t-\epsilon/2) + \epsilon a(t), \\ a(t) &= -x(t). \end{aligned} \tag{9.16}$$





Newton's *Principia*, Book I, Theorem I

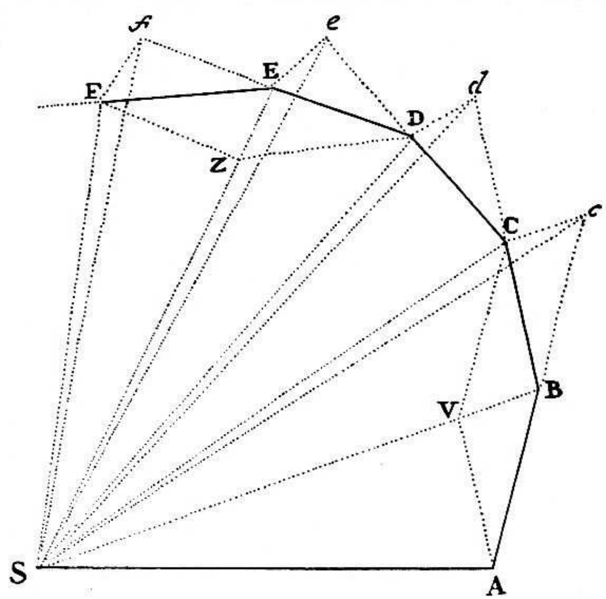
SECTION II

The determination of centripetal forces.

PROPOSITION I. THEOREM I

The areas which revolving bodies describe by radii drawn to an immovable centre of force do lie in the same immovable planes, and are proportional to the times in which they are described.

For suppose the time to be divided into equal parts, and in the first part of that time let the body by its innate force describe the right line AB. In the second part of that time, the same would (by Law 1), if not hindered,



proceed directly to *c*, along the line B*c* equal to AB; so that by the radii AS, BS, *c*S, drawn to the centre, the equal areas ASB, BS*c*, would be described. But when the body is arrived at B, suppose that a centripetal force acts at once with a great impulse, and, turning aside the body from the right line B*c*, compels it afterwards to continue its motion along the right line BC.

The leapfrog method. . .

- is simple
- is fast
- is relatively accurate
- is time-reversible
- preserves momentum and angular momentum
- has no drift of energy
- preserves quasiperiodic orbits [KAM tori]
- produces qualitatively correct chaotic orbits
- is symplectic

Channel & Scovel, 1990

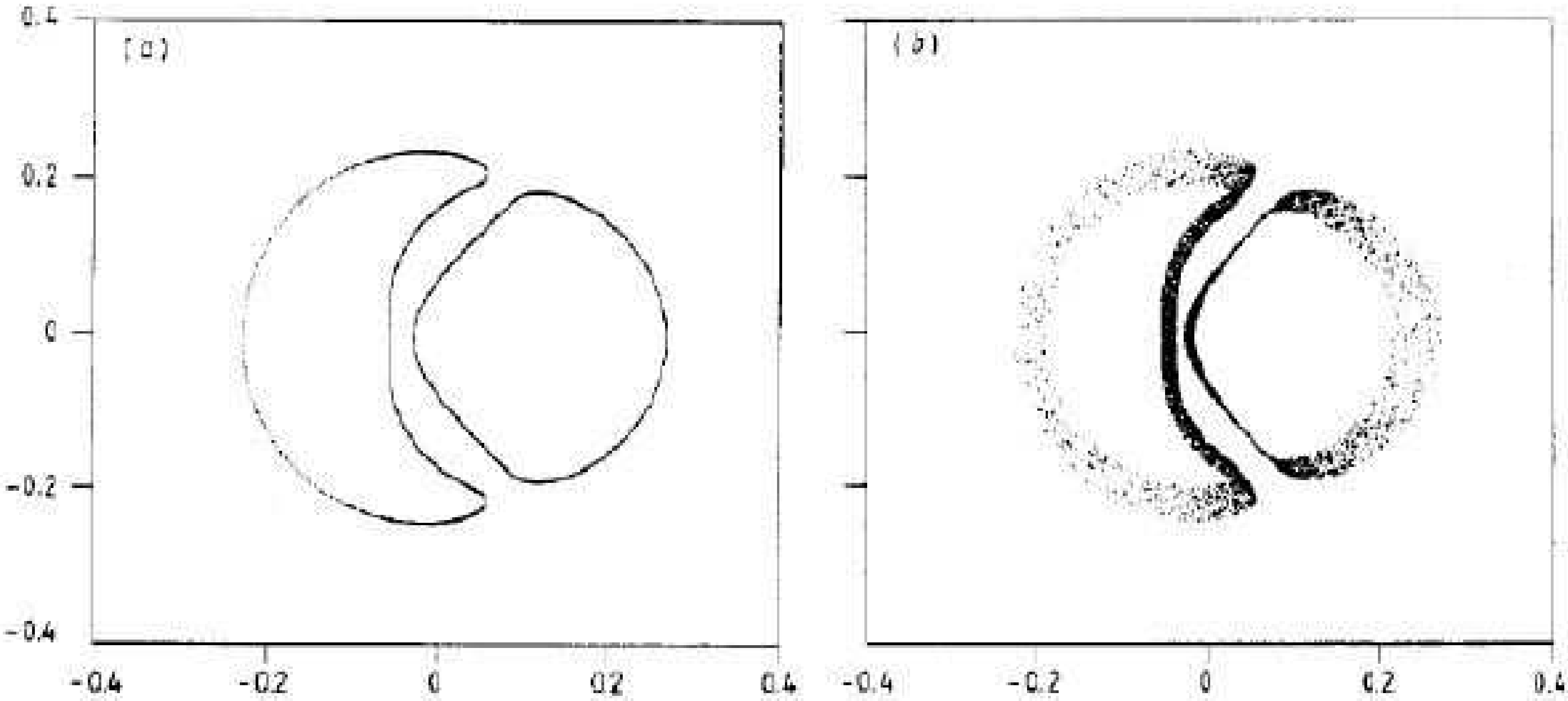
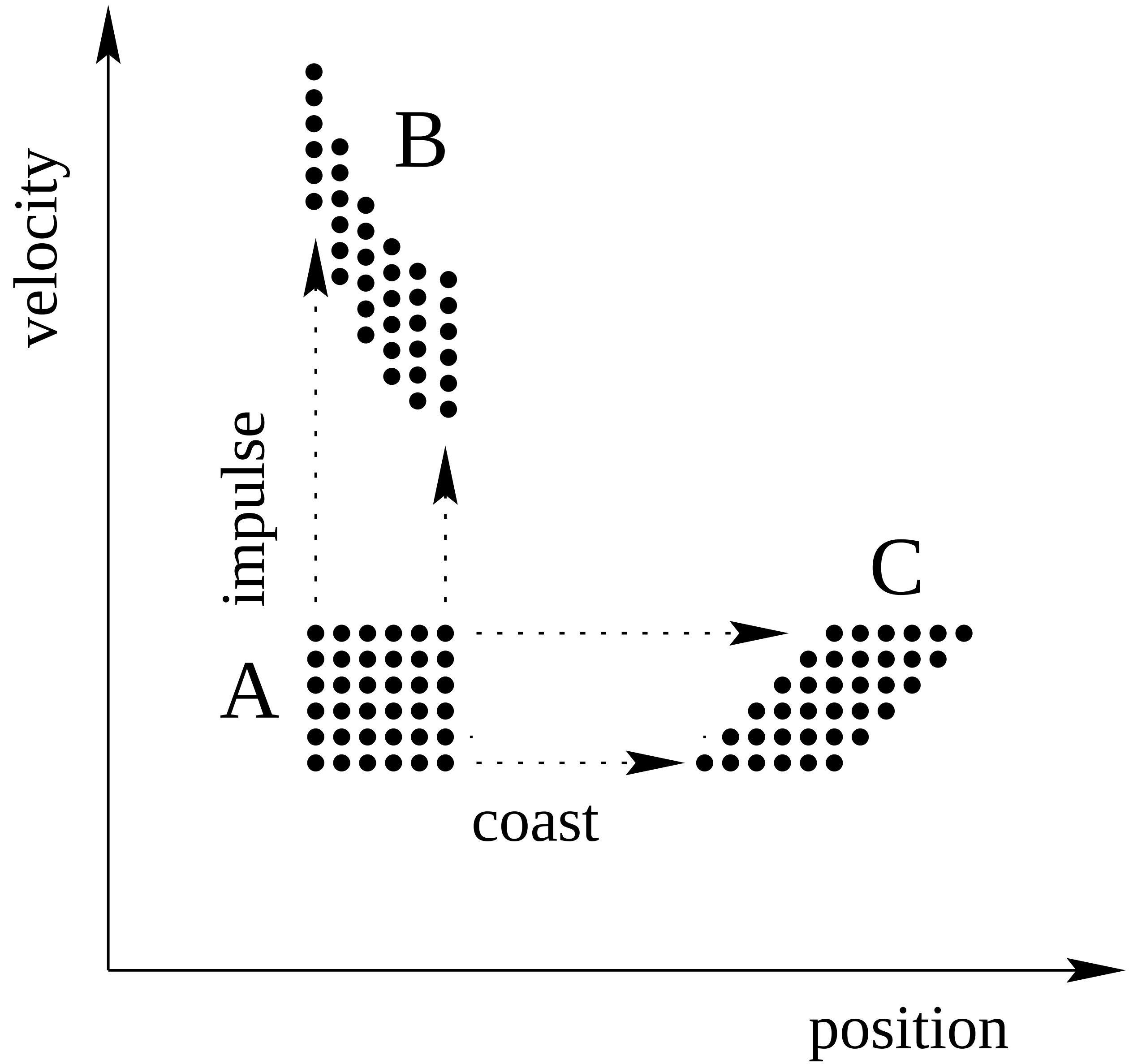


Figure 2. Comparison of third-order SIA (*a*) and a fourth-order RKI (*b*) for the Hénon–Heiles system. The initial condition was (0.12, 0.12, 0.12, 0.12) and energy 0.029 952. The timestep was 1/6 and 1200 000 timesteps were computed.

What is symplecticity?

- Phase space T^*Q carries a symplectic 2-form ω
- Flow of Hamilton's equations $i_X\omega = -dH$ satisfies $\exp(tX)^*\omega = \omega$
- The leapfrog method also satisfies $\varphi^*\omega = \omega$

What is symplecticity?

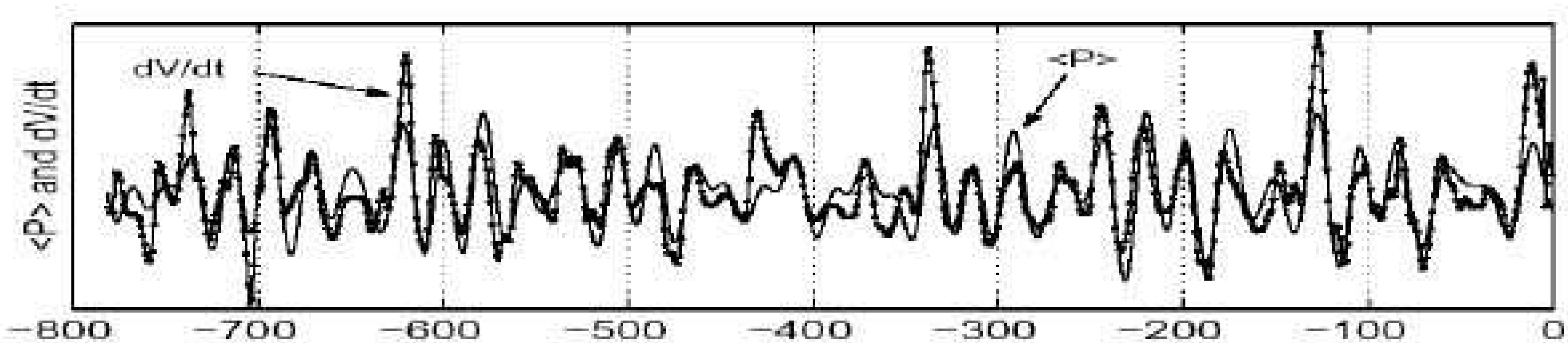


Missed opportunities

Freeman Dyson

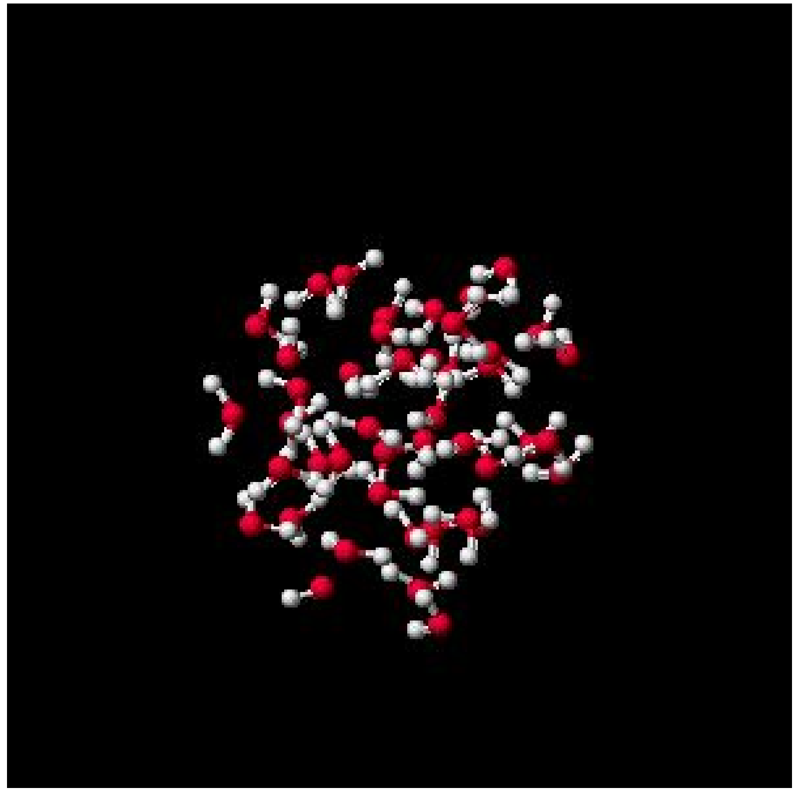
"I am acutely aware of the fact that the marriage between mathematics and physics, which was so enormously fruitful in past centuries, has recently ended in divorce."

The ice ages explained



(Sverker Edvarddson 2002)

Simulation of cold water



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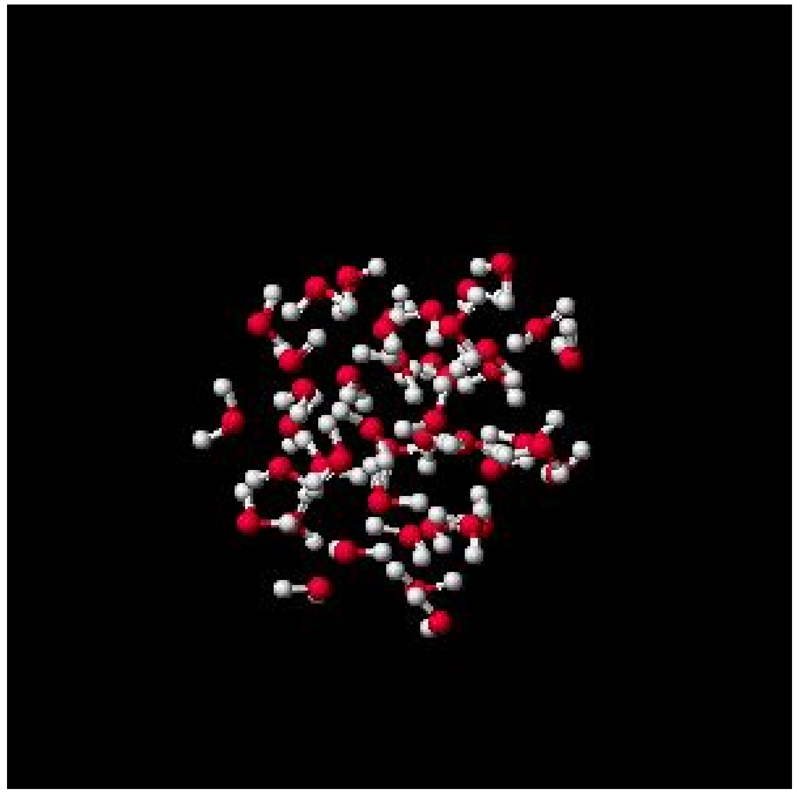

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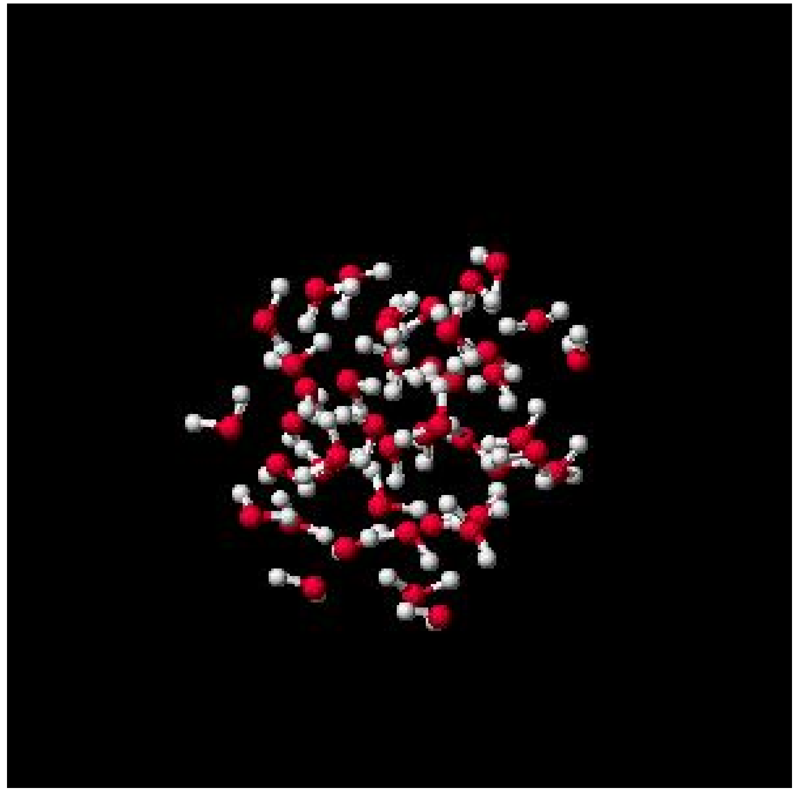

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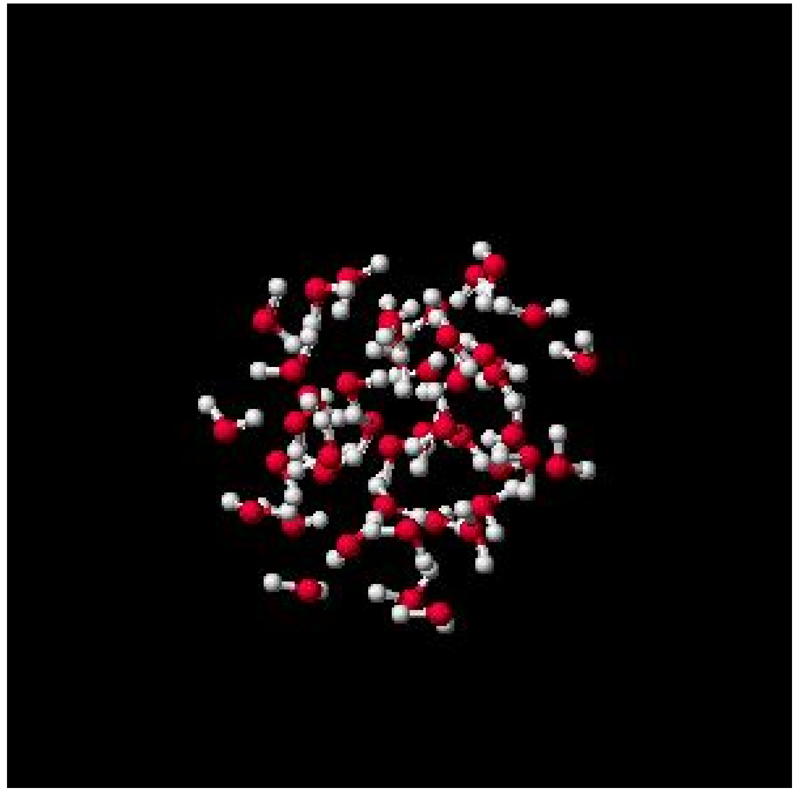

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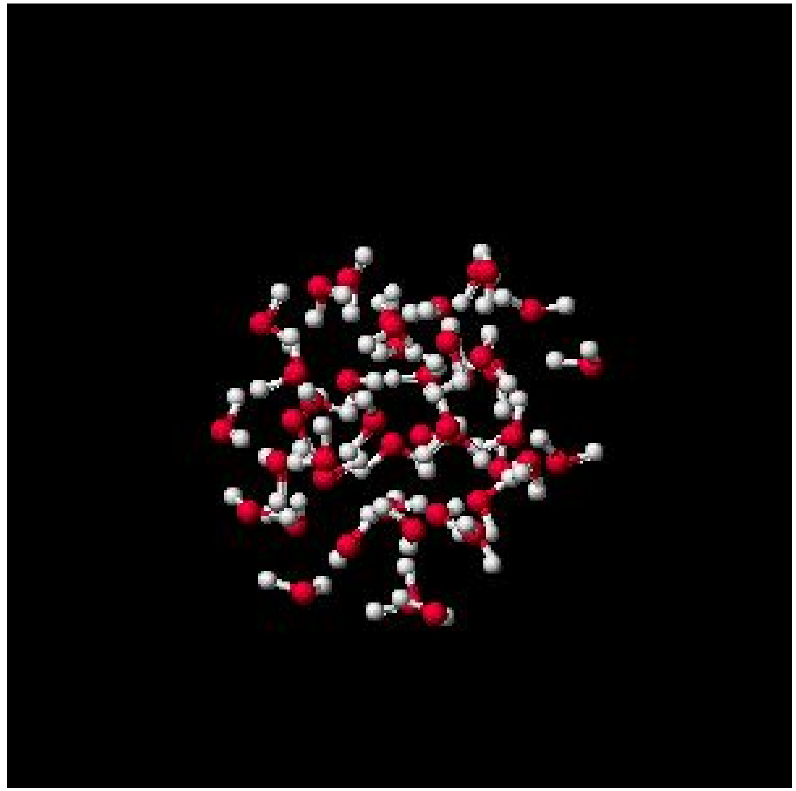

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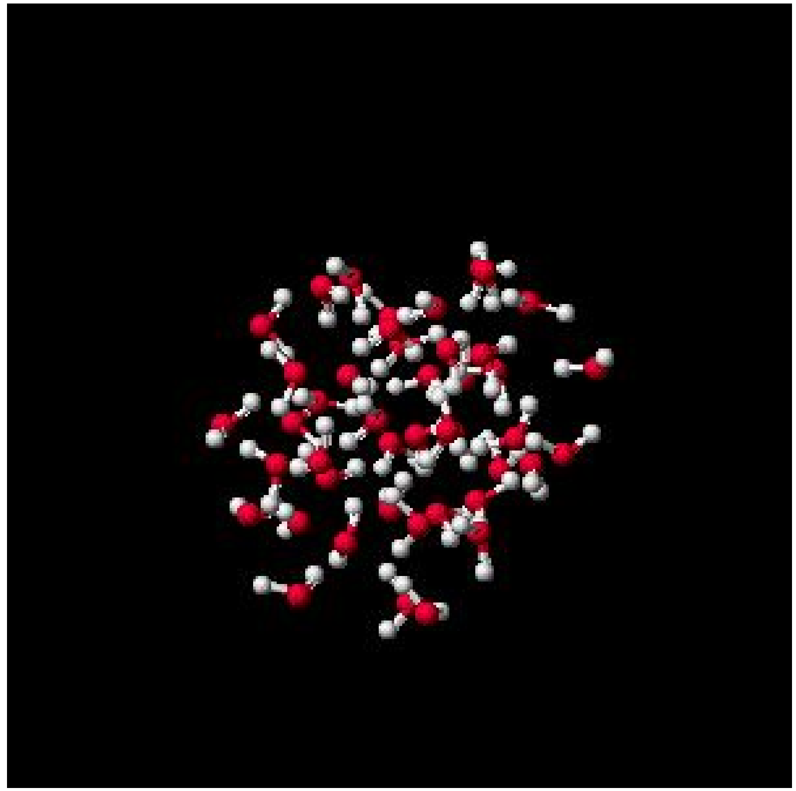

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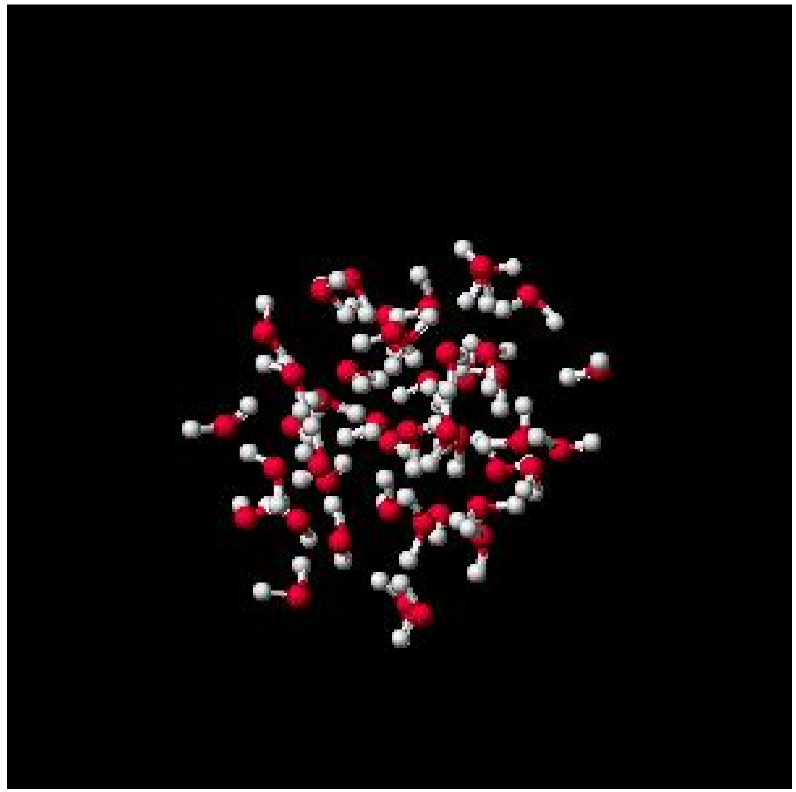

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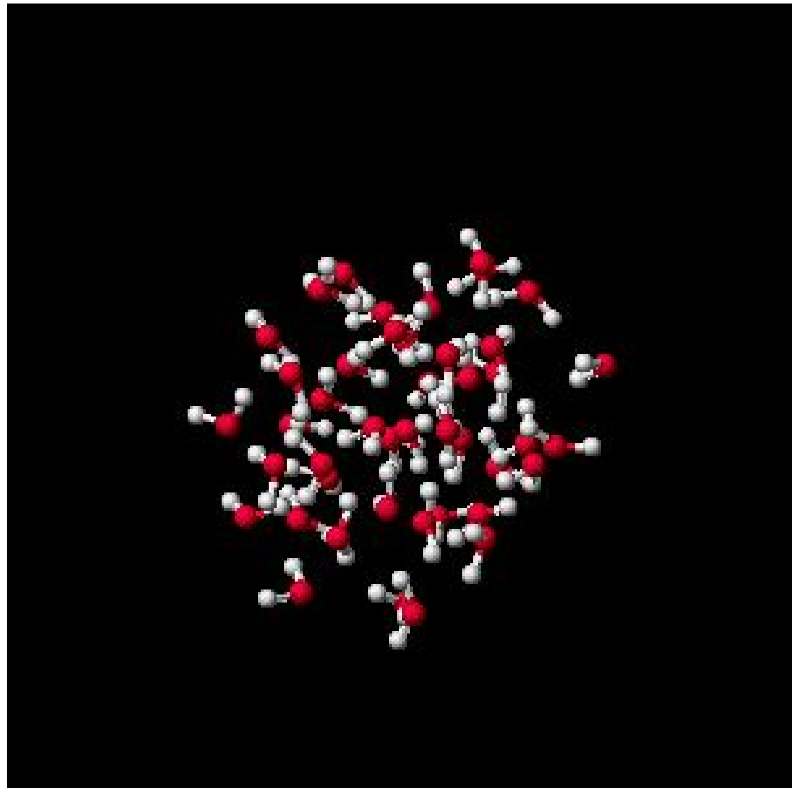

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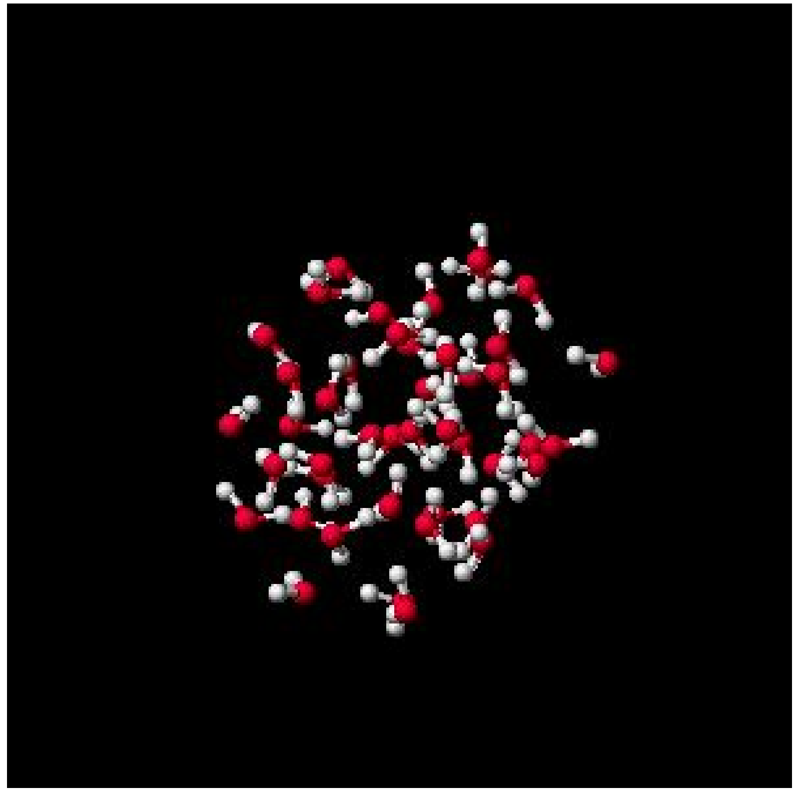

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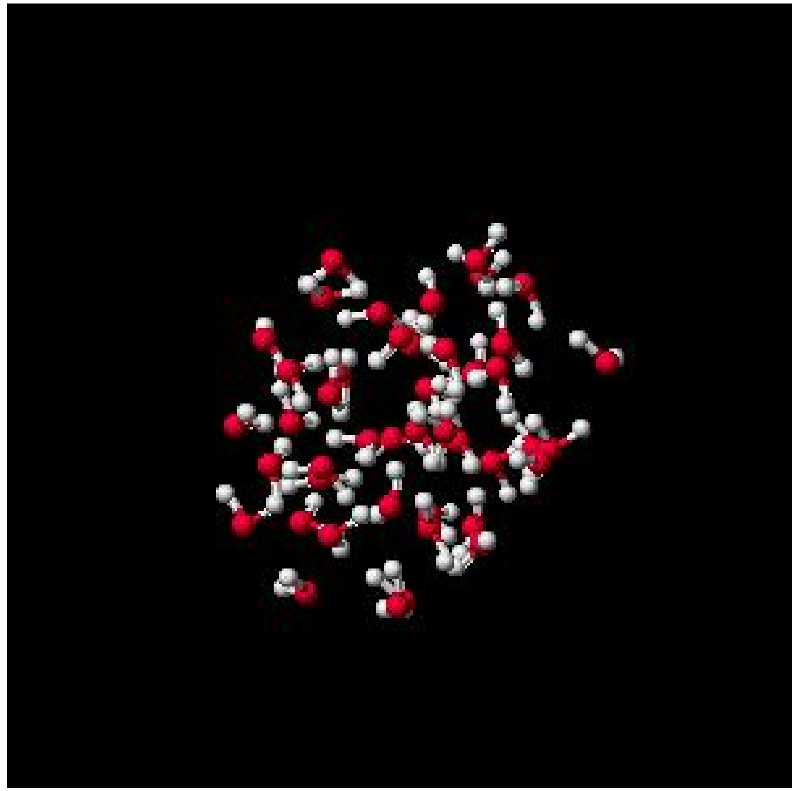

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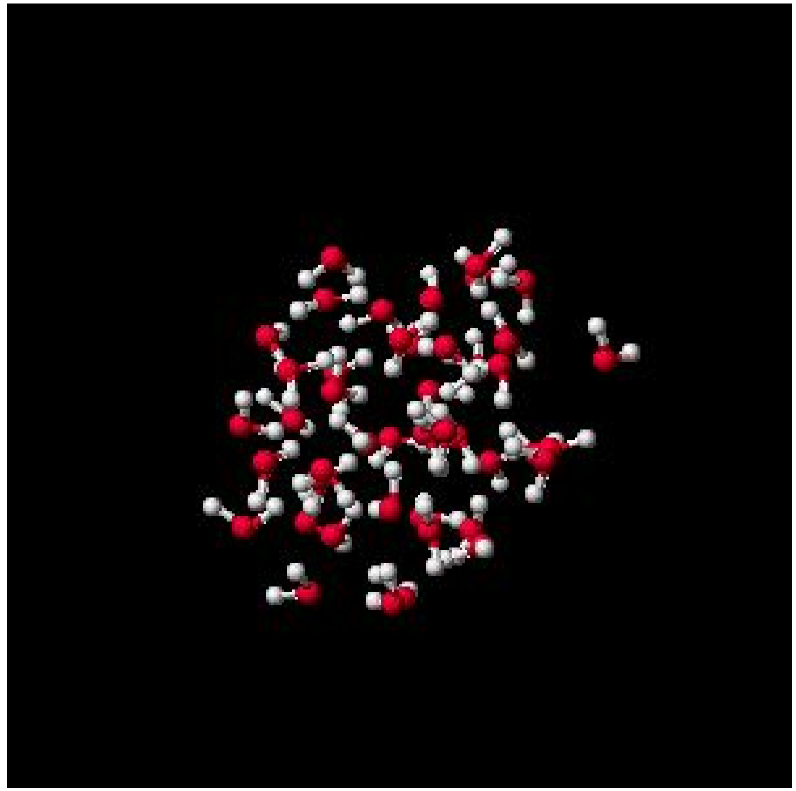

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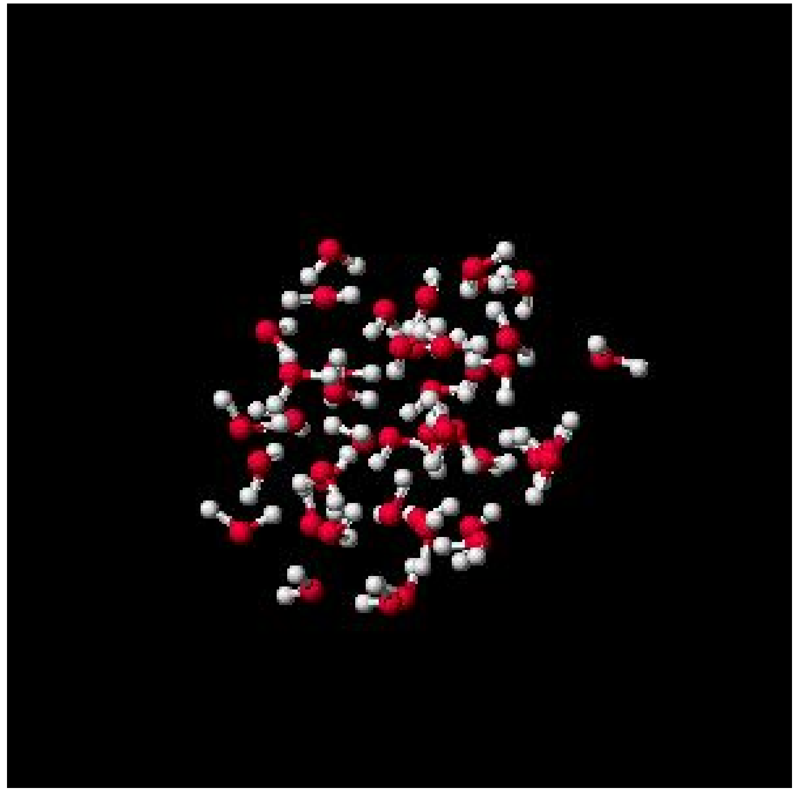

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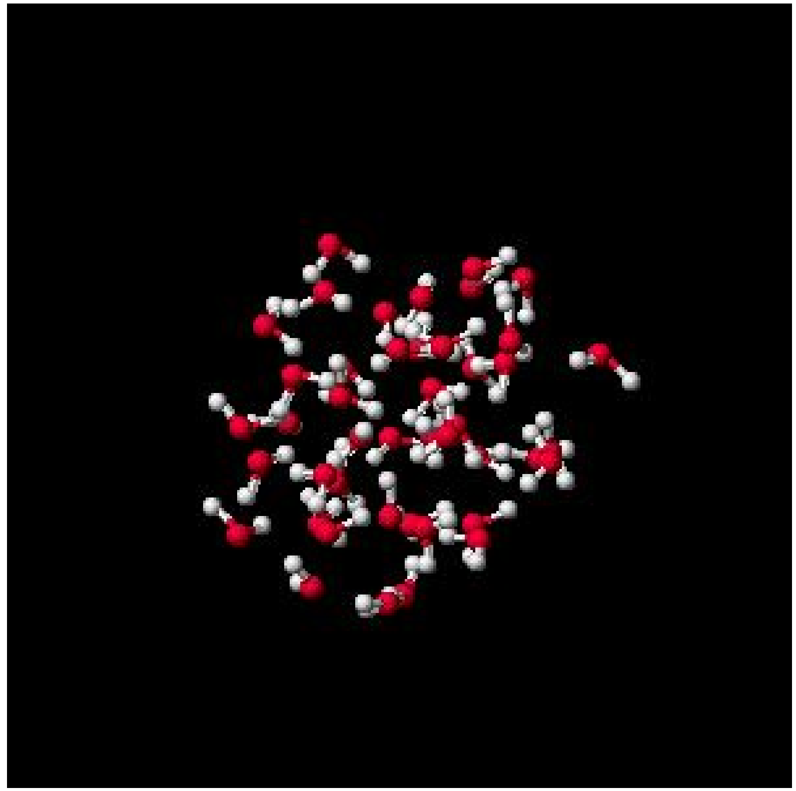
Simulation of cold water



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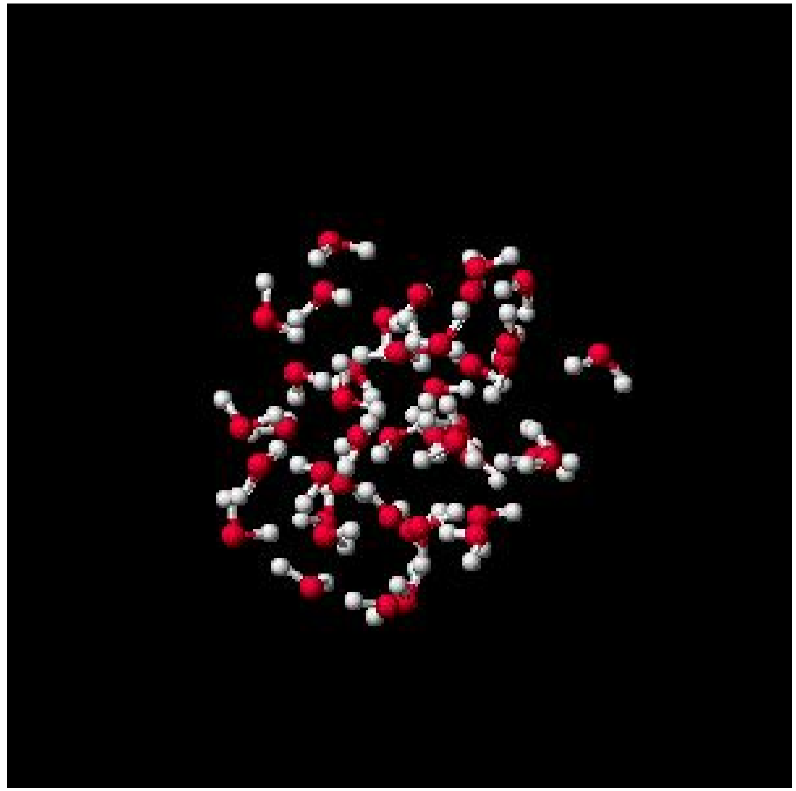
Simulation of cold water



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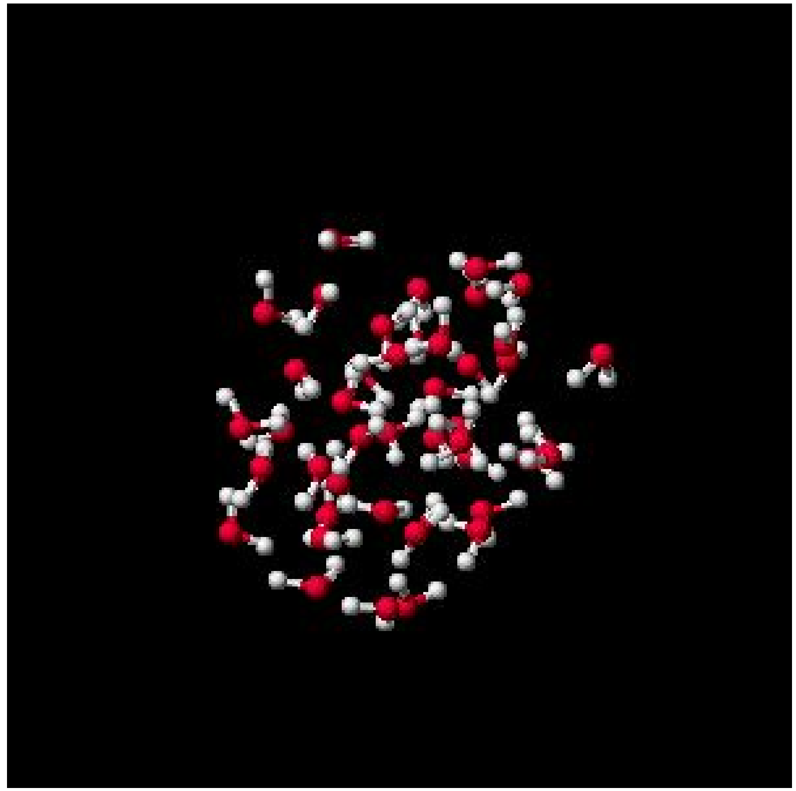

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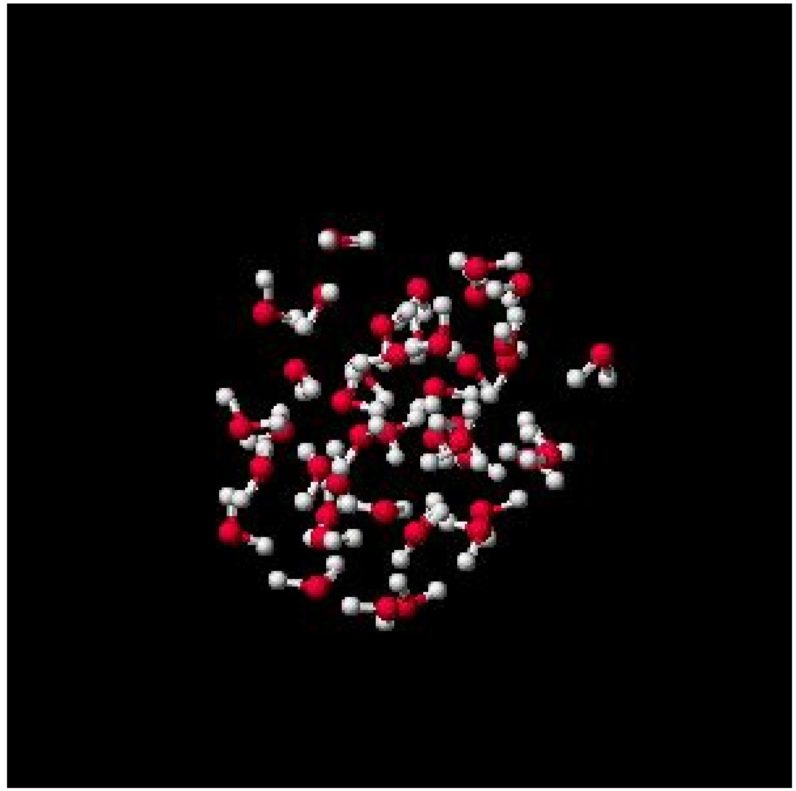

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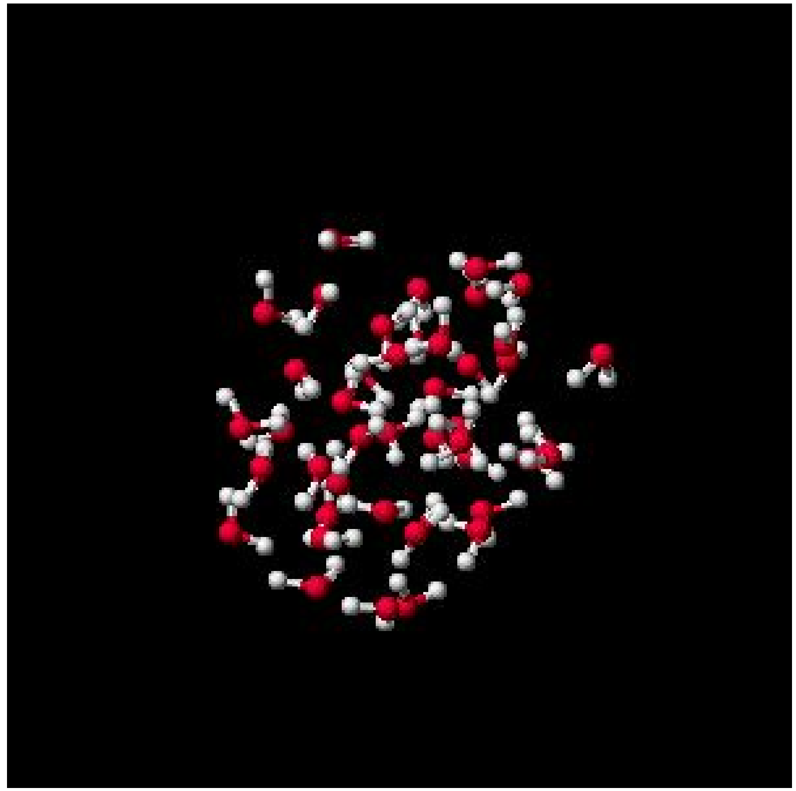

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Backward error analysis

Let $\mathcal{G}$ be a set of diffeomorphisms with a tangent space G at the identity. Let $\varphi = 1 + (\Delta t)X + o(\Delta t) \in \mathcal{G}$. Then

- If $\varphi \in C^r$ then there exists $\widetilde{X} \in G$ such that $\varphi = \exp(\Delta t\widetilde{X}) + \mathcal{O}((\Delta t)^r)$
- If φ is analytic then $\varphi = \exp(\Delta t\widetilde{X}) + \mathcal{O}(e^{-a/\Delta t})$.

Therefore properties generic to G are (almost) preserved.

For example, let $\mathcal{G}$ = symplectic maps, G=Hamiltonian vector fields. Then symplectic integrators have bounded energy errors for exponentially long times $\mathcal{O}(e^{a/\Delta t})$.

Splitting methods

Let $X = \sum_{i=1}^{n} X_i$ with $X, X_i \in G$. Use the integrators

$$\varphi_1(\Delta t) = \exp(\Delta t X_1) \circ \ldots \exp(\Delta t X_n)$$

$$\varphi_2(\Delta t) = \varphi_1(\Delta t/2)\varphi_1^{-1}(-\Delta t/2)$$

$$\varphi_4(\Delta t) = \varphi_2(z\Delta t)\varphi_2((1-2z)\Delta t)\varphi_2(z\Delta t), \quad z = (2-2^{1/3})^{-1}$$

where

$$\varphi_j = \exp\left(\Delta t X + \mathcal{O}((\Delta t)^{j+1})\right).$$

Requires knowing

- an explicit form (generating function) for all $X \in G$
- a way of constructing lots of integrable $X_i \in G$.
- the Baker-Campbell-Hausdorff formula
  $\exp(A)\exp(B) = \exp\left(A + B + \frac{1}{2}[A,B] + \frac{1}{6}[A,[A,B]] + \ldots\right)$

Analysis of splitting methods

Quickly leads to studying $L(X_1, X_2, \ldots)$, the free Lie algebra generated by the X_i.

Simplest and most common case: split the Hamiltonian $H = T + V = \frac{1}{2}pM(q)p + V(q)$ and study $L(T, V)$.

This Lie algebra is not free, because T is quadratic in p, leading to $[V,[V,[V,T]]] \equiv 0$.

It is $L_{\mathfrak{P}}(T, V)$, the Lie algebra of classical mechanics.

Polynomial gradings

Definition. A Lie algebra L is of class $\mathfrak{P}$ ('polynomially graded') if it is graded, i.e. $L_{\mathfrak{P}} = \bigoplus_{n\geq 0} L_n$, and its homogeneous subspaces L_n satisfy

$$[L_n, L_m] \subseteq L_{n+m-1} \text{ if } n > 0 \text{ or } m > 0\text{; and}$$

$$[L_0, L_0] = 0$$

We call the grading of L its grading by degree.

$L_{\mathfrak{P}}(T, V)$ also has the standard grading by order (= number of Lie brackets + 1), which satisfies $L_{\mathfrak{P}} = \bigoplus_{m>0} L^m$ and

$$[L^n, L^m] \subseteq L^{n+m}.$$

The Lie algebra of classical mechanics

Theorem.

$$L_{\mathfrak{P}}(T,V) = \mathcal{Z} \oplus L(T,[T,\mathcal{Z}])$$

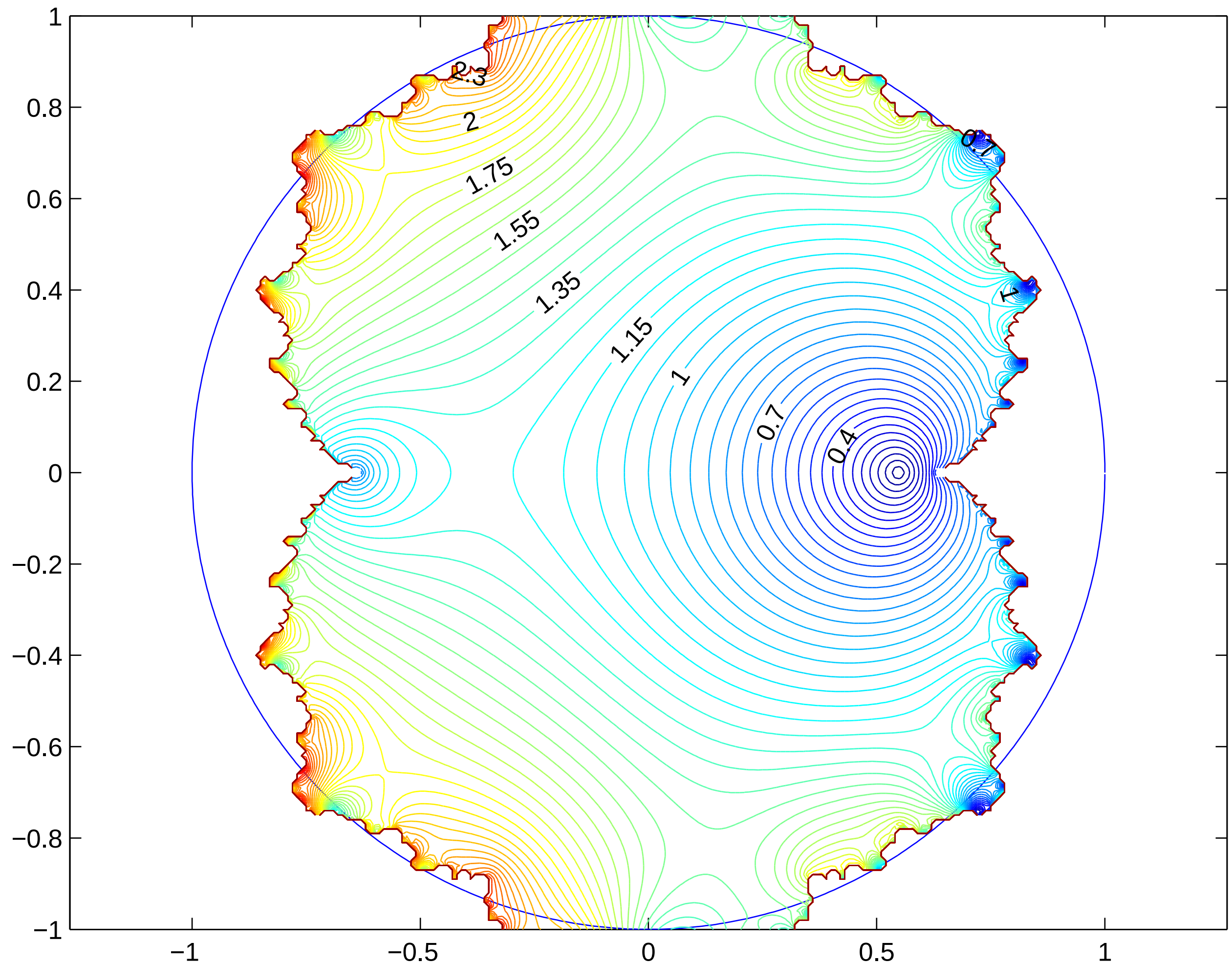
where $\mathcal{Z} = \{V,[V,[V,T]],\ldots\}$ is an infinite set of degree–0 (potential energy) functions.

$$\dim L^n_{\mathfrak{P}}(T,V) \sim \frac{1}{n}\alpha^n,$$

where $\alpha = 1.82542377420108\ldots$ is the entropy of classical mechanics.

(Recall that in the free case, $\dim L^n(A,B) \sim \frac{1}{n}2^n$ (Witt 1936).)

GF for CM



$\left|e^{x(t)}\right|$ where $x(t) = \sum_{n=0}^{\infty} \dim L^n_{\mathfrak{P}}(T,V) t^n$.

Classification of dynamical systems

Sets of dynamical systems can form a

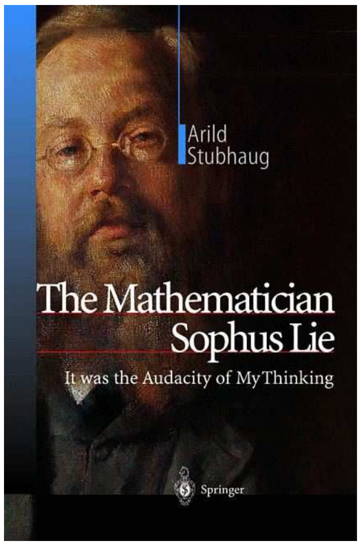
- semigroup (examples: systems with Lyapunov functions, systems which contract volume)
- symmetric space closed under $(\varphi, \psi) \mapsto \varphi\psi^{-1}\varphi$ (example: maps with a reversing symmetry $\varphi^{-1} = R\varphi R^{-1}$)
- group (examples: all diffeomorphisms, symplectic maps, volume-preserving maps)

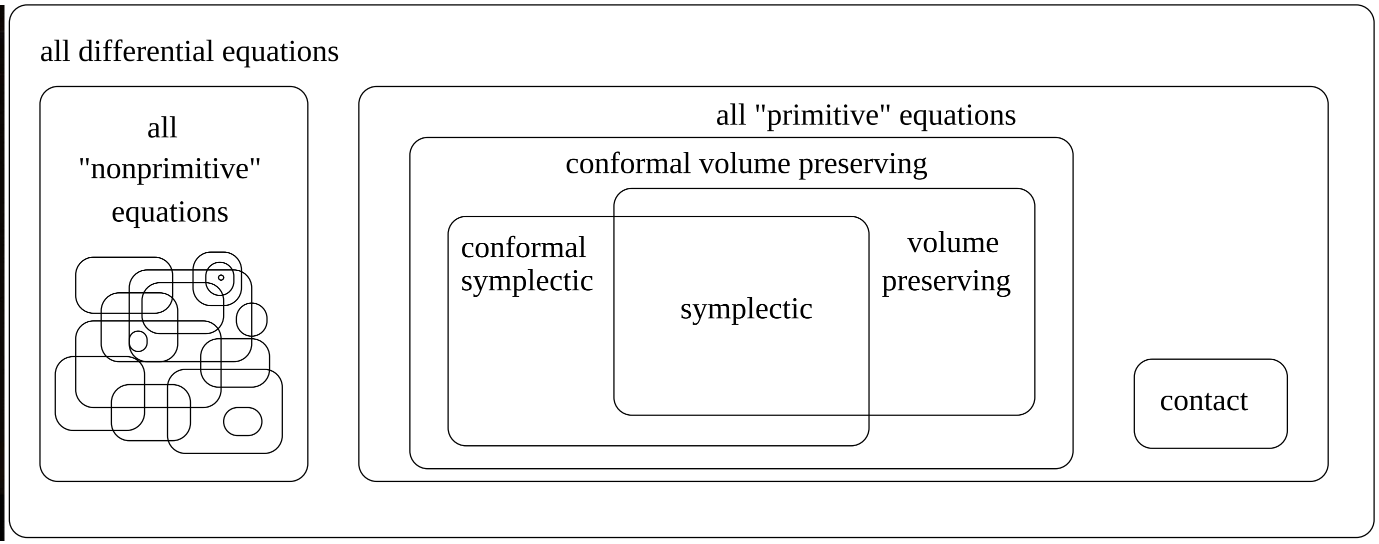
with linearizations to a Lie wedge, Lie triple, and Lie algebra respectively.

The big picture

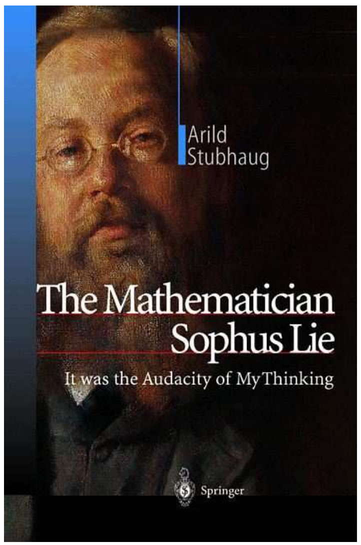
1. to find all groups, semigroups, and symmetric spaces of diffeomorphisms
2. to find their normal forms
3. to find a way to detect the structure in a given system
4. to study their relationships under intersection
5. to study the dynamics of their perturbations
6. to determine the characteristic dynamics and invariants of each class
7. to develop good (i.e. simple, fast, stable) integrators for each class

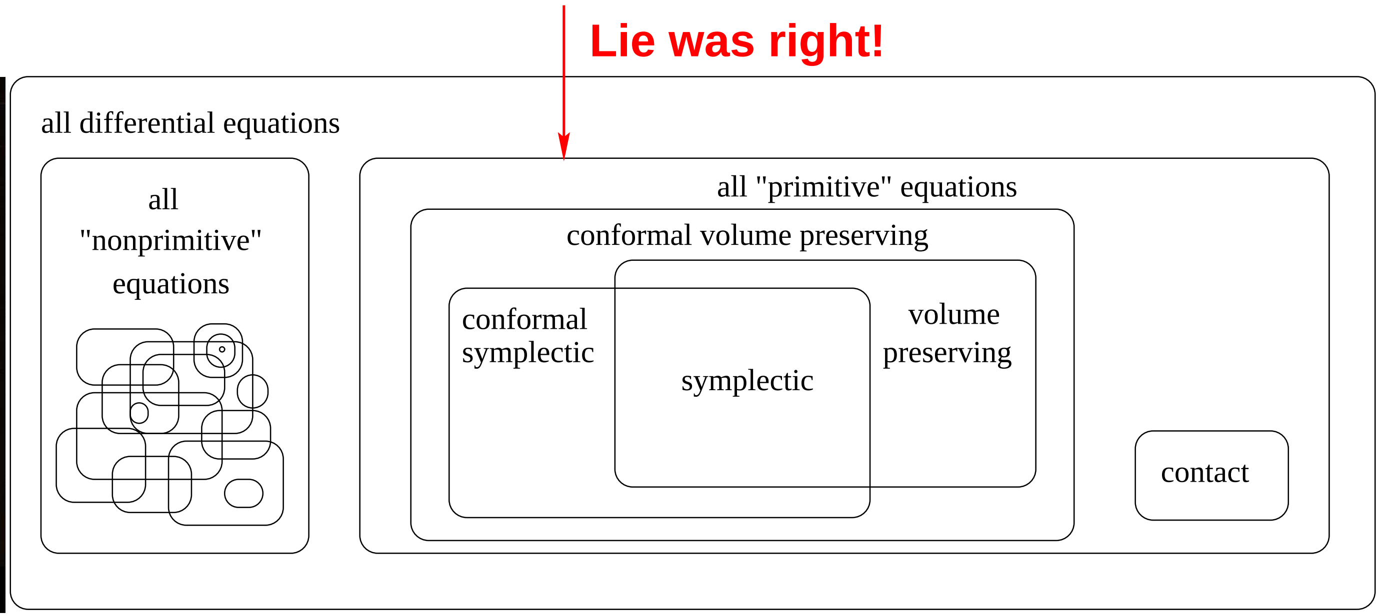
What was known in 1895





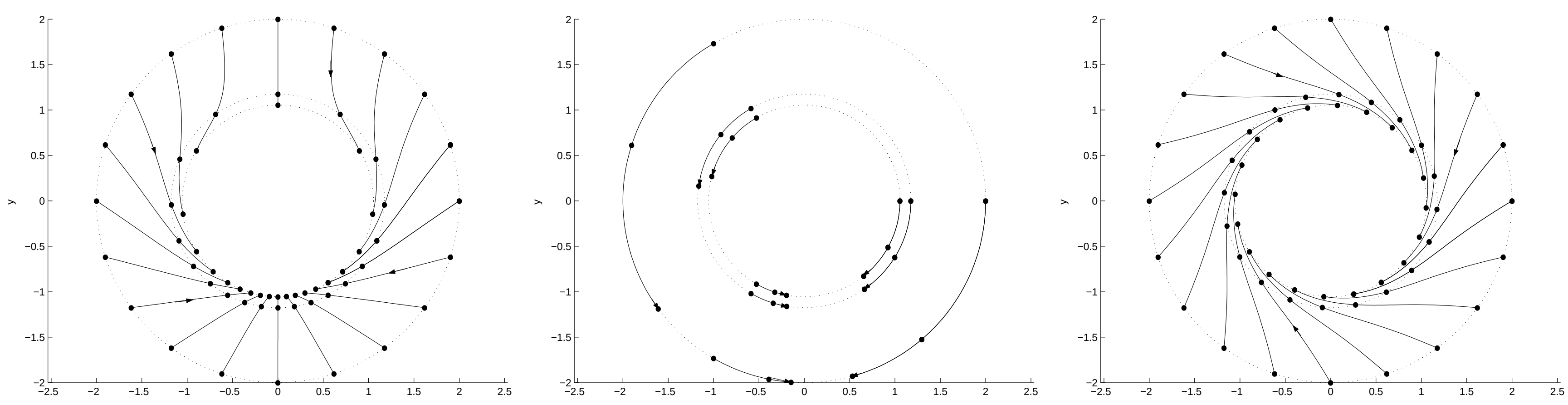
What is known in 2003





Nonprimitive groups of diffeomorphisms

- preserve some foliation of phase space (leaves map to leaves)
- may preserve some (e.g. symplectic) structure on the leaves
- may preserve some structure on the space of leaves
- may have some complicated interaction between the leaves and the leaf space



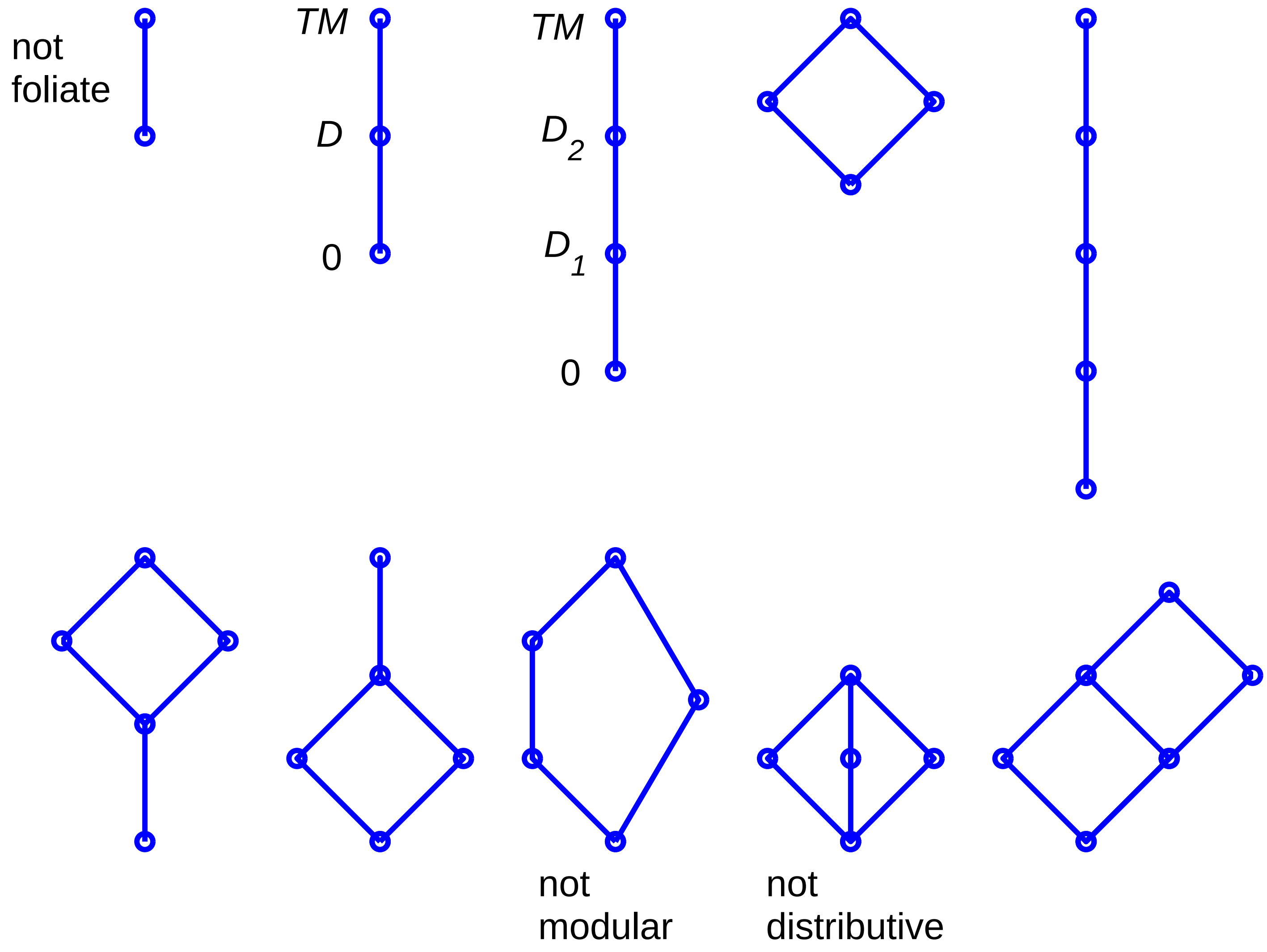
Example

Let G be a Lie group acting on the Poisson manifold $(P, \{,\})$. Let $H : P \to$ be a G-invariant Hamiltonian. Its flow preserves 4 foliations:

1. the level sets of H
2. the level sets of the momentum map of G
3. the symplectic leaves of P
4. the orbits of G

More generally, a diffeomorphism φ on a manifold M can preserve any set of foliations, which must contain $\emptyset$, M, and be closed under intersections and joins. That is, the set of foliations forms a lattice (generalizes Kodaira & Spencer 1961).

Lattices with ≤ 3 foliations



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Thank you for your attention!