Let's imagine... computational physics algorithms *... (for) the future*

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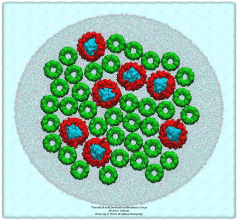
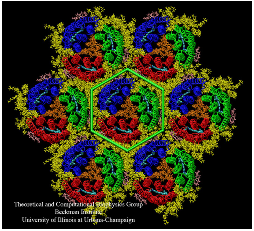
Example 1: Molecular dynamics

Simulation of **huge** mechanical systems (10^8 atoms) over **long times.**





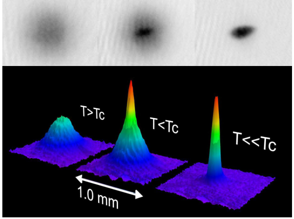
Photosynthetic membrane of a purple bacterium, purple membrane
Images: K. Schulten, Urbana-Champain & LIA with C. Chipot (Nancy)

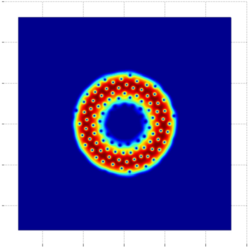
Sources of error:

- Modelling error,
- Time integration,
- Computation of the potential (space discretization)

Example 2: Bose-Einstein condensates

Bosons gases at very low temperature develop macroscopic stable structures. Simulation of 3D **nonlinear Schrödinger equations .**





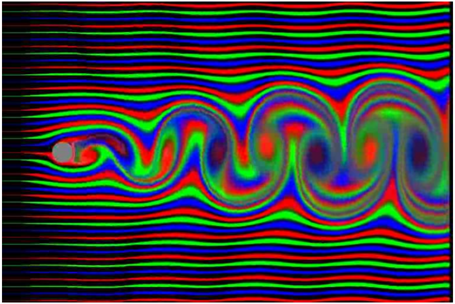
Images: W. Ketterle and D. Pritchard at MIT; X. Antoine at U. Nancy & INRIA

Sources of error:

- Time integration.
- Space discretization: 2D or 3D grids, use of CFL conditions.
- Non-linear instabilities.

Example 3: Euler equation in fluid mechanics

Describe the motion of two-dimensional fluids
Von Kármán vortex streets: Real life *vs.* numerical simulation

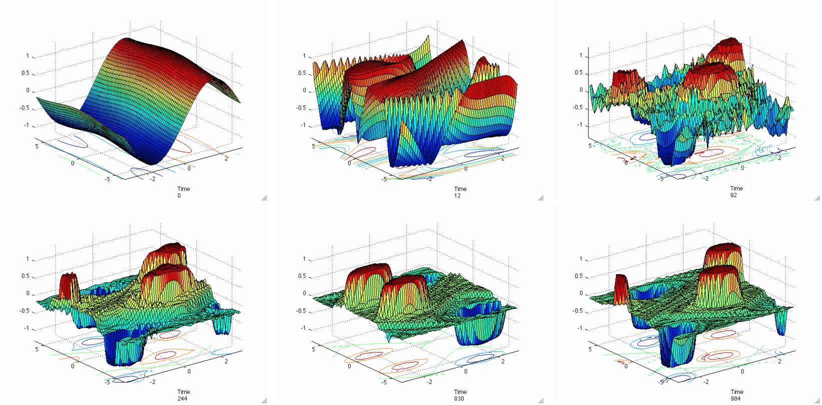



Sources of error:

- Time and space discretization: semi-lagrangian schemes
- Non-linear instabilities (turbulence)

Example 3: Euler equation in fluid mechanics

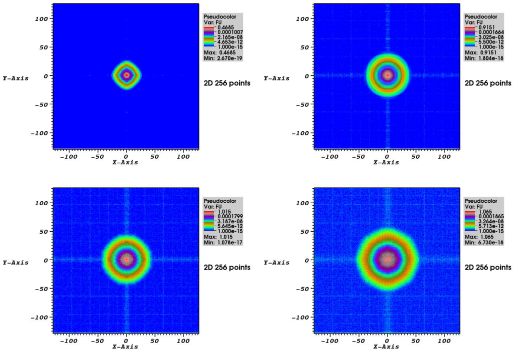
Simulation of the 2D Euler equation: help to find **quasiperiodic solutions**



N. Crouseilles & E. Faou, *Quasiperiodic solution to the 2D Euler equations*, 2012.

Example 4: Weak-turbulence in quantum mechanics

Schrödinger system: **existence of energy cascades?**



Computational issues:

- Long time simulations needed (with R. Belaouar (CMAP))
- No parallel solver for time evolution problems.

A mathematical model

Toy problem in dimension d ($= 1$ or 10^8). $y \in \mathbb{C}^d$.

$$\dot{y} = i\omega y + y^2$$

- i reflects the mechanical structure (oscillations)
- $\omega >> 1$ high frequencies of the system
- y^2: nonlinear interactions.

Linear part: $y(t) = \exp(-i\omega t) y(0)$ *high oscillations*

Non-linear part: $y(t) = \alpha/(t - t_*)$ *blow-up*

Change of variable: $z(t) = \exp(-i\omega t) y(t)$.

$$\dot{z}(t) = z(t)^2 e^{i\omega t}$$

A mathematical model

$$\dot{z}(t) = z(t)^2 e^{i\omega t} \Longrightarrow z(t) = z(0) + \int_0^t z(s)^2 e^{i\omega s} \mathrm{d}s.$$

Integration by part:

$$\begin{aligned}
\int_0^t z(s)^2 e^{i\omega s} \mathrm{d}s &= \frac{1}{i\omega} \int_0^t z(s)^2 \Big(\frac{\mathrm{d}}{\mathrm{d}s} e^{i\omega s}\Big) \mathrm{d}s \\
&= -\frac{1}{i\omega} \int_0^t e^{i\omega s} \Big(\frac{\mathrm{d}}{\mathrm{d}s} z(s)^2\Big) \mathrm{d}s + \frac{1}{i\omega} \Big[z(s)^2 e^{i\omega s}\Big]_0^t \\
&= \mathcal{O}\big(\frac{1}{\omega}\big) << 1
\end{aligned}$$

High oscillations stabilize the system.

$$y(t) \simeq \exp(-i\omega t) y(t) + \mathcal{O}\big(\frac{1}{\omega}\big)$$

A fundamental phenomenon in nonlinear waves evolutions.

Numerical resonances

$$\dot{z}(t) = z(t)^2 e^{i\omega t}$$

Numerical integration: h small, $z(nh) \simeq z_n$ given by

$$\frac{z_{n+1} - z_n}{h} = z_n^2 e^{i\omega h n}$$

Numerical resonances: $e^{i\omega h} \simeq 1$. Averaging fails.

- Problem very generic. Arises in all applications.
- Numerical scheme: an important tool to discover and analyze nonlinear physical and mathematical phenomena
- It is fundamental to extensively study the mathematical properties of numerical algorithms for themselves.

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Let's imagine the future... of mathematics in a digital world