Structure preserving algorithms for differential equations; Applications computing and education

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eScience meeting, Geilo, Jan. 2007

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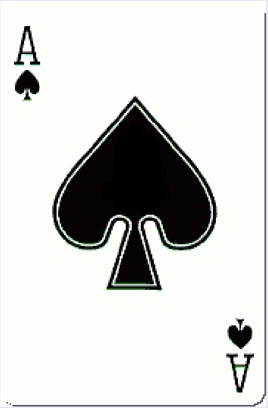
SpadeAce



Formulation of Differential Equations

Concrete approach: (HOW?)

- Coordinate presentations.
- Focusing on quantitative information and solution algorithms.
- Usual approach in *Applied Mathematics*.

Abstract approach: (WHAT?)

- Coordinate free formulations.
- Focusing on *geometric* and *qualitative* features .
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Mind the Gap!

- The Gap opened and widened during 20'th century.
- Developments in last decade contribute to a narrowing of the gap.

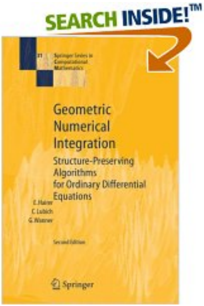
Two Legs of SpadeAce ♠

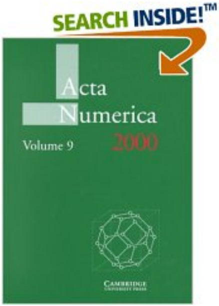
Geometric Integration

- Mostly time integration.
- Early ref: DeVogelaire (1955).
- Systematic theory Feng Kang (1980s).
- Recognized international research activity 1990s.
- Norway: Trondheim & Bergen groups.

Compatible Discretizations

- Space discretization.
- Early ref.: Whitney (1957).
- Systematic theory: Bossavit (1980s).
- Norway: Oslo group.





One LEG: Geometric Integration

Example 1: Hamiltonian equations

The solar system:

- q, p : position and momentum, 6 variables.
- H : Hamiltonian function (total energy).

$$H = V(q) + p^T p/2m \quad \text{(kinetic and potential energy)}$$

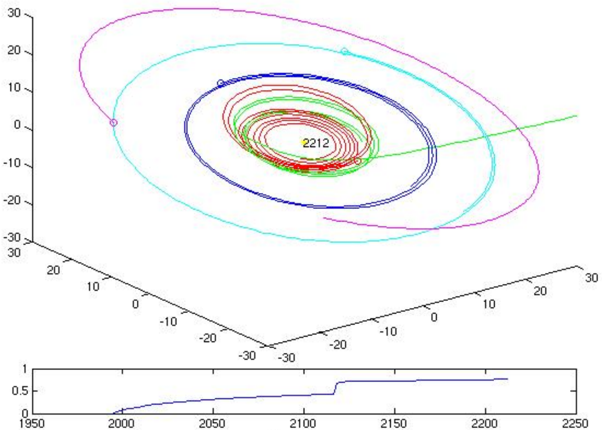
Equations in Hamiltonian form:

$$\frac{\partial q}{\partial t} = \frac{\partial H}{\partial p}$$

$$\frac{\partial p}{\partial t} = -\frac{\partial H}{\partial q}$$

Three methods:

1. Eulers method: $y_{n+1} = y_n + hF(y_n)$.
2. Inverse Euler: $y_{n+1} = y_n + hF(y_{n+1})$.
3. Symplectic Euler: Euler on q, inverse Euler on p.



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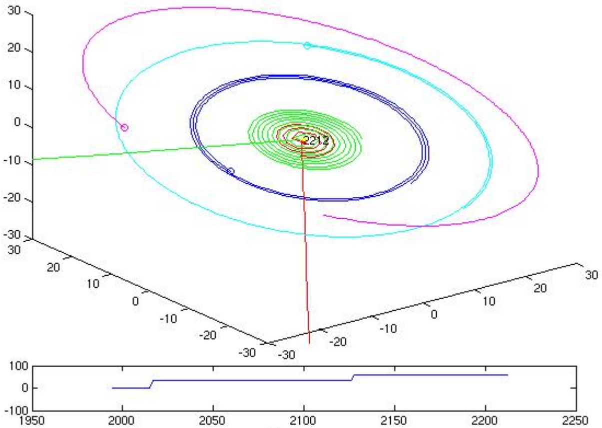

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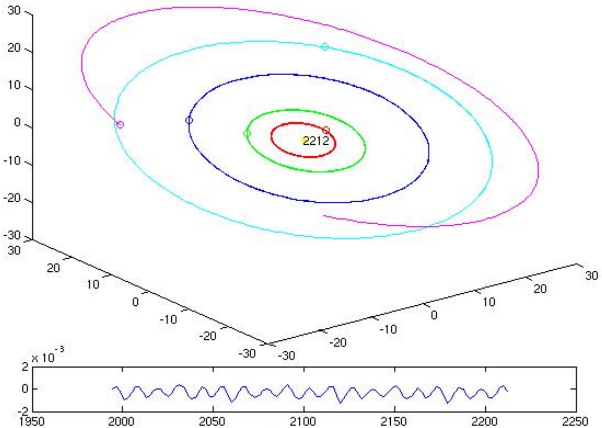

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Note:

- All methods used the same timestep $h = 10$ days.
- All errors are equal (per step), $\mathcal{O}(h^2)$.
- Only the last method preseves the *symplectic structure*.

Symplectic method.

$\Downarrow$

The methods solves *exactly*:

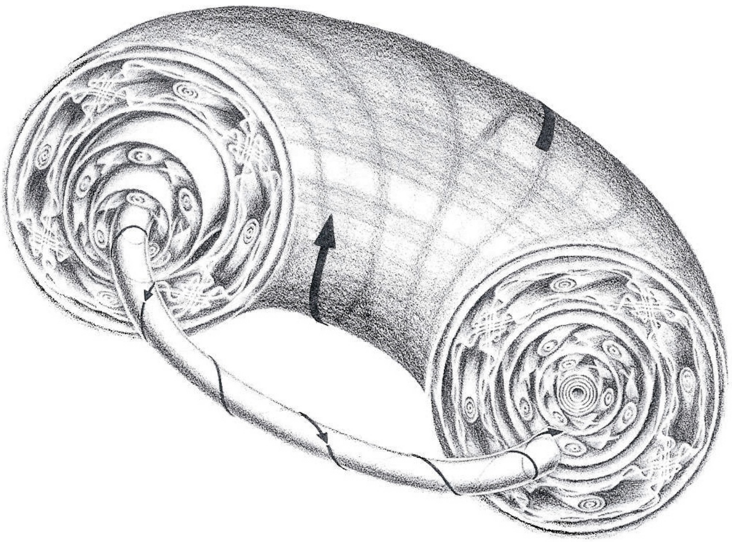
Modified Hamiltonian equations:

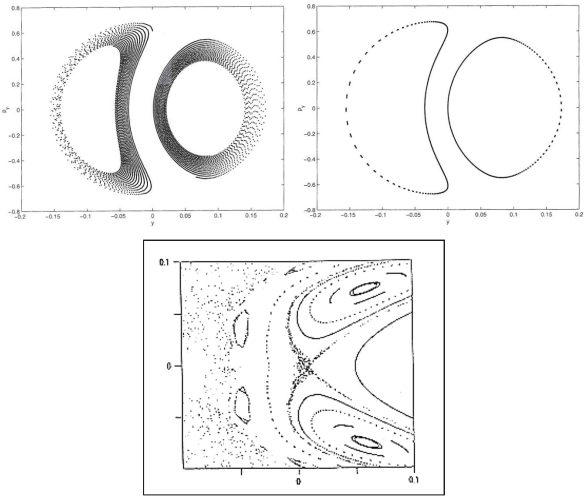
$$\frac{\partial q}{\partial t} = \frac{\partial \tilde{H}}{\partial p}$$

$$\frac{\partial p}{\partial t} = -\frac{\partial \tilde{H}}{\partial q}$$

where $\tilde{H} \approx H$.

Kolmogorov - Arnol'd - Moser (KAM) theory





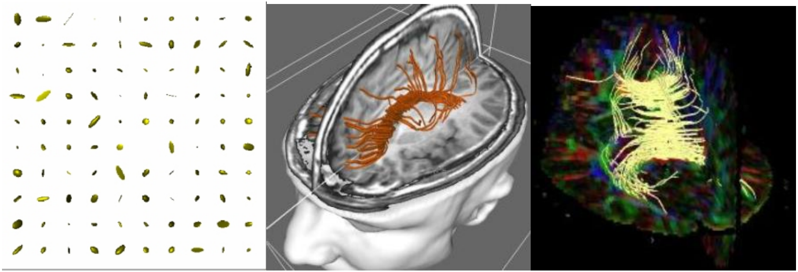
Geometric Integrators:

- Symplectic integrators (Hamilt. ODEs).
- Multisymplectic integrators (Hamilt. PDEs).
- Variational integrators, discrete Lagrangians.
- Lie-Poisson integrators.
- Energy and momentum preserving schemes.
- Methods preserving first integrals.
- Volume preserving integrators.
- Lie group integrators.

Methods which *exactly* preserve an underlying structure $\Rightarrow$

- Qualitative better properties at long time integration.
- Higher accuracy in each step.
- Backwards error analysis (structure preservation).
- Physical 'soundness' of numerical model.

Ex3: Regularizing Diffusion Tensor Images



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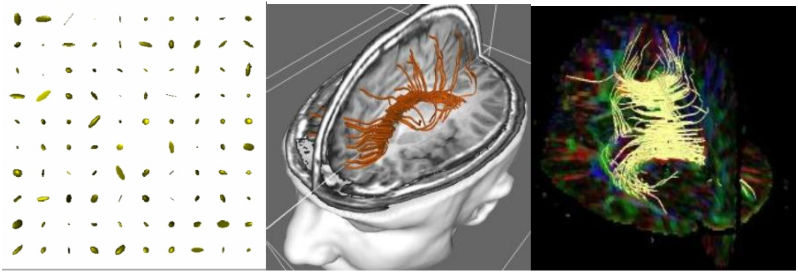

Problem

How to regularize data without destroying Symmetric Positive Definiteness of Diffusion Tensor?

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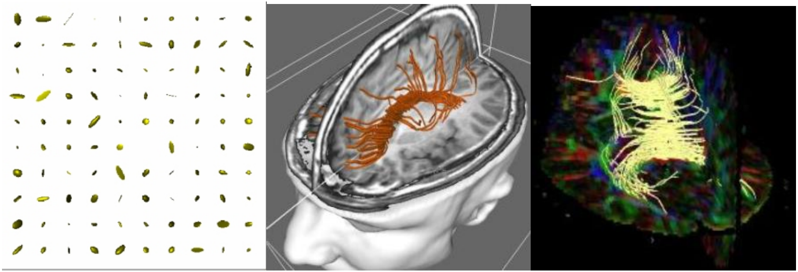

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Solution (Aubert, Faugeras & al.: Use Lie group method)

Update with similarity transforms: $Y_{n+1} = Q(\ldots)Y_nQ(\ldots)^{-1}$.

The other LEG: Compatible Discretizations

deRahm Cohomology

$$\mathbb{R} \hookrightarrow \Lambda^0(\Omega) \xrightarrow{d} \Lambda^1(\Omega) \xrightarrow{d} \cdots \xrightarrow{d} \Lambda^n(\Omega) \to 0$$

d: exterior derivative, $d^2 = 0$.

Special case: $\Omega = \mathbb{R}^3$:

$$\mathbb{R} \hookrightarrow C^\infty(\Omega, \mathbb{R}) \xrightarrow{\text{grad}} C^\infty(\Omega, \mathbb{R}^3) \xrightarrow{\text{curl}} C^\infty(\Omega, \mathbb{R}^3) \xrightarrow{\text{div}} C^\infty(\Omega, \mathbb{R}) \to 0$$

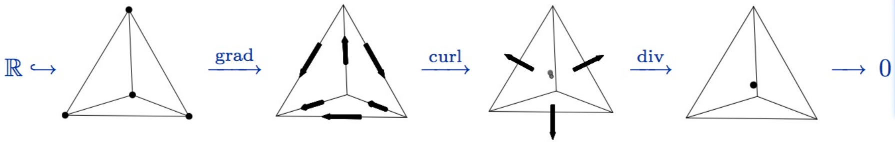
Stokes' theorem (Green, Gauss, ..., and the whole gang):

$$\int_\Omega d\mu = \int_{\partial\Omega} \mu.$$

Discrete cohomology and Mixed finite elements

Arnold–Winther theory:

$$
\begin{array}{ccccccccccc}
\mathbb{R} \hookrightarrow & C^\infty(\Omega,\mathbb{R}) & \xrightarrow{\text{grad}} & C^\infty(\Omega,\mathbb{R}^3) & \xrightarrow{\text{curl}} & C^\infty(\Omega,\mathbb{R}^3) & \xrightarrow{\text{div}} & C^\infty(\Omega,\mathbb{R}) & \longrightarrow & 0 \\
 & \downarrow & & \downarrow & & \downarrow & & \downarrow & & \\
\mathbb{R} \hookrightarrow & W_h & \xrightarrow{\text{grad}} & Q_h & \xrightarrow{\text{curl}} & S_h & \xrightarrow{\text{div}} & V_h & \longrightarrow & 0
\end{array}
$$



- Unifies and explaines families of mixed finite elements.
- Stability theory for elasticity.

Principal objectives SpadeAce ♠:

- Join national and international research efforts within *Compatible Discretizations* and *Geometric Integration* for PDEs, to develop new algorithms and software.
- Pursue hard computational challenges in application areas selected from elasticity, fluid flows, Schrödinger equations and field equations of mathematical physics.
- Establish an interdisciplinary network for training and exchange of PhD students.
- Maintain the international excellence of Norwegian research in structure preserving computational techniques in the next decade.

Participants

Norwegian nodes:

- **UiB Bergen:** Prof. Hans Munthe-Kaas, Associate professor Antonella Zanna, Post Doc Roman Kozlov, Post Doc Ilan Degani, PhD stud. NN.
- **UiO Oslo:** Associate Professor Snorre Christiansen, Professor Ragnar Winther, PhD student Tore G Halvorsen, PhD student NN.
- **NTNU Trondheim:** Prof. Brynjulf Owren, Associate professor Elena Celledoni, Post Doc David Cohen, PostDoc Xavier Raynaud, PhD stud. NN.
- **SINTEF Applied Mathematics Trondheim:** Senior Scientist Trond Kvamsdal.

Participants (cont.)

International nodes:

- **Austin Texas**: Prof. Tom J.R. Hughes.
- **Minneapolis:** Prof. Douglas N. Arnold.
- **Pavia**: Professor Annalisa Buffa.
- **Potsdam:** Professor Sebastian Reich.
- **Surrey/Kent:** Professor Peter Hydon, Professor Elizabeth Mansfield.
- **Tübingen:** Professor Christian Lubich, Professor Jörg Frauendiener.

Project info

Project period

Jan. 2007 - Dec. 2011 (5 years).

Budget

1.9 mill NoK pro anno.

Personnel:

2 x 2 year Post Doc.,

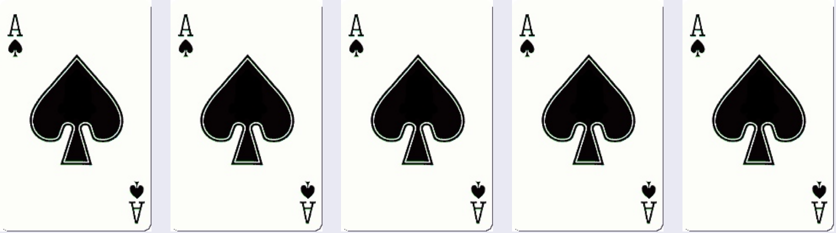
2 x 3 year PhD stud.

Sub–goals SpadeAce ♠:

- Extend informal annual MAGIC (Manifolds and Geometric Integration Colloquia) workshops to a wider format.
- Organize one larger international meeting on Structure Preserving Algorithms for Differential Equations in Norway, following up on the Minnesota '04 and Oslo '05 meetings.
- Publication of research papers, software and a research monograph.
- Visits of short and long duration by students and researchers between participating nodes.
- Two PhD candidates (3 years) and two postdocs (2 years).
- Creation of web-resources for information on the research progress. Extension of the FoCM Geometric Integration Interest Group `www.focm.net/gi` to include resources on compatible discretizations.

Coming Soon to a Theatre Near You:

SpadeAce - the movie



http://spadeace.uib.no