Some geometrical aspects in shell theory and in numerical integration of hamiltonian systems

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Shell theory

What is shell theory?

Thin shell:

$$S \times (-\varepsilon, \varepsilon) \ni (\mathrm{P}, x_3) \mapsto P + x_3 \mathbf{n}(\mathrm{P}) \in \Omega^\varepsilon$$

S surface of $\mathbb{R}^3$, $\mathbf{n}(\mathrm{P})$ normal to S in P . Plate: $S \subset \mathbb{R}^2$.

Lateral boundary: $\Gamma^\varepsilon = \partial S \times (-\varepsilon, \varepsilon)$. Upper and lower faces $S \times \{\pm\varepsilon\}$.

Three dimensional displacement $\mathbf{u} = (\mathrm{u}_1, \mathrm{u}_2, \mathrm{u}_3)$ in Cartesian coordinates.
Strain tensor

$$e_{ij}(\mathbf{u}) = \frac{1}{2}\Big(\frac{\partial \mathrm{u}_i}{\partial x_j} + \frac{\partial \mathrm{u}_j}{\partial x_i}\Big).$$

Isotropic material

$$A^{ijkl} = \lambda \delta^{ij} \delta^{kl} + \mu(\delta^{ik}\delta^{jl} + \delta^{il}\delta^{jk}),$$

λ and μ Lamé constants.

$$a^\varepsilon(\mathbf{u}, \mathbf{u}') = \int_{\Omega^\varepsilon} A^{ijk\ell} e_{ij}(\mathbf{u}) e_{k\ell}(\mathbf{u}') \mathrm{d}\mathbf{x}$$

What is shell theory ?

$V(\Omega^\varepsilon) = \{\mathbf{u} \in H^1(\Omega^\varepsilon)^3 \,|\, \mathbf{u}|_{\Gamma^\varepsilon} = 0\}$. (Clamped boundary conditions)

Problem with loading:

Find $\mathbf{u}^\varepsilon \in V(\Omega^\varepsilon)$ *such that*
$$a^\varepsilon(\mathbf{u}^\varepsilon, \mathbf{u}') = \int_{\Omega^\varepsilon} \mathbf{f}^\varepsilon \cdot \mathbf{u}' \,\mathrm{d}\mathbf{x}, \quad \forall \mathbf{u}' \in V(\Omega^\varepsilon)$$

Eigenmode problem:

Find $\mathbf{u}^\varepsilon \in V(\Omega^\varepsilon)$, $\mathbf{u}^\varepsilon \neq 0$, *and* $\Lambda^\varepsilon \in \mathbb{R}$ *such that*
$$a^\varepsilon(\mathbf{u}^\varepsilon, \mathbf{u}') = \Lambda^\varepsilon \int_{\Omega^\varepsilon} \mathbf{u}^\varepsilon \cdot \mathbf{u}' \,\mathrm{d}\mathbf{x}, \quad \forall \mathbf{u}' \in V(\Omega^\varepsilon)$$

Behavior of $\mathbf{u}^\varepsilon$ and/of Λ^ε as $\varepsilon \to 0$?

Three dimensional energy: $\mathrm{E}_{3\mathrm{D}}[\mathbf{u}] = a^\varepsilon(\mathbf{u}, \mathbf{u})$.

Two-dimensional models

Orthogonal coordinates, $(x_\alpha, x_3) \in S \times (-\varepsilon, \varepsilon)$
The displacement is written (u_α, u_3) $(\alpha = 1, 2)$.

Two dimensional models:

$$\mathbf{K}(\varepsilon) = \mathbf{M} + \varepsilon^2 \mathbf{B}$$

acting on two-dimensional displacements (z_α, z_3).
M membrane operator, **B** bending operator.

Controversial in the sixties: what is the *best* model?
[Koiter (1959-1970), Naghdi (1963), Budianski & Sander (1967)]

Limit of u as $\varepsilon \to 0$ idenfied in the 90's
[Sanchez-Palencia (1990), Ciarlet, Lods & Miara (1996)]

Koiter's operator

- **M** is a 2D elasticity operator associated with the membrane strain tensor

$$\gamma_{\alpha\beta}(\mathbf{z}) = \frac{1}{2}(\mathrm{D}_\alpha \mathrm{z}_\beta + \mathrm{D}_\beta \mathrm{z}_\alpha) - b_{\alpha\beta}\mathrm{z}_3$$

$b_{\alpha\beta}$ curvature tensor. $\mathrm{D}_\alpha = \partial_\alpha + \dots$ covariant derivative.

- **B** is a 2D elasticity operator associated with the change of curvature tensor:

$$\rho_{\alpha\beta}(\mathbf{z}) = \mathrm{D}_\alpha \mathrm{D}_\beta \mathrm{z}_3 - b_\alpha^\sigma b_{\sigma\beta}\mathrm{z}_3 + b_\alpha^\sigma \mathrm{D}_\beta \mathrm{z}_\sigma + \mathrm{D}_\alpha b_\beta^\sigma \mathrm{z}_\sigma.$$

- Orders of derivative: $\mathbf{K}(\varepsilon)$ acts on (z_α, z_3).

$$\mathbf{M} + \varepsilon^2 \mathbf{B} = \begin{pmatrix} 2 & 1 \\ 1 & 0 \end{pmatrix} + \varepsilon^2 \begin{pmatrix} 2 & 3 \\ 3 & 4 \end{pmatrix}$$

Two dimensional energy $\mathrm{E}^\varepsilon_{2\mathrm{D}}[\mathbf{z}]$.

Koiter estimate (1970)

- Solution of the Koiter model:

$$\mathbf{K}(\varepsilon)\mathbf{z} = \frac{1}{2\varepsilon}\int_{-\varepsilon}^{\varepsilon} \mathbf{f}^{\varepsilon}(\mathrm{x}_3)\mathrm{d}\mathrm{x}_3.$$

- Reconstruction operator

$$\mathbf{Uz} = \begin{cases} \mathrm{z}_\sigma - \mathrm{x}_3(\mathrm{D}_\sigma \mathrm{z}_3 + 2b_\sigma^\alpha \mathrm{z}_\alpha) + \mathrm{x}_3^2\, b_\sigma^\alpha \theta_\alpha(\mathbf{z}), \\ \mathrm{z}_3 - p\,\mathrm{x}_3 \gamma_\alpha^\alpha(\mathbf{z}) + p\,\frac{\mathrm{x}_3^2}{2}\rho_\alpha^\alpha(\mathbf{z}), \end{cases}$$

with $p = \lambda/(\lambda + 2\mu)$ and $\theta_\sigma(\mathbf{z}) = \mathrm{D}_\sigma \mathrm{z}_3 + b_\sigma^\alpha \mathrm{z}_\alpha$.

Uz defines a 3D displacement polynomial in x_3.

Koiter estimate (1970)

$$\mathrm{E}^{\varepsilon}_{3\mathrm{D}}[\mathbf{u} - \mathbf{U}\mathbf{z}] \leq C_S\Big(\frac{\varepsilon^2}{L^2} + \frac{\varepsilon}{R}\Big)\mathrm{E}^{\varepsilon}_{2\mathrm{D}}[\mathbf{z}].$$

- $\mathbf{u}$ solution of the three-dimensional equations.
- $1/R$ the maximum principal curvature of S.
- L involved in inverse estimates of derivatives of $\mathbf{z}$.

$$\|\mathrm{D}\gamma(\mathbf{z})\| \leq L^{-1}\|\gamma(\mathbf{z})\| \quad \text{and} \quad \|\mathrm{D}\boldsymbol{\rho}(\mathbf{z})\| \leq L^{-1}\|\boldsymbol{\rho}(\mathbf{z})\|$$

- Adimensional estimate
- L may depend on ε.
- Methods used by Koiter: averaging the 3D equations.

Complete asymptotics

When they are available, complete asymptotic expansions of the displacements **u** and **z** allow to give optimal estimates.

Strategy:

- Expand the three dimensional operator in powers of ε with intrinsic coefficients (tensors on S).
- Obtain a reduced 2D model in formal series.
- Solve the formal series with boundary conditions (Boundary layer terms).
- Obtain optimal bounds by using a priori estimates.

Clamped elliptic shells

PhD Work.

1. E. Faou, CRAS (2000) and (2001).
2. E. Faou, *Elasticity on a thin shell: Formal series solution*, Asymptotic Analysis, (2002).
3. E. Faou, *Multiscale expansions for linear clamped elliptic shells*, Comm. in PDE (2004).

S elliptic means that the Gaussian curvature is posive.

Example: spherical cap.

Clamped elliptic shells

Complete asymptotic expansion in powers of $\sqrt{\varepsilon}$:

$$\mathbf{u}^{\varepsilon} \simeq (\mathbf{v}^0 + \boldsymbol{\varphi}^0) + \varepsilon^{1/2}(\mathbf{v}^{1/2} + \boldsymbol{\varphi}^{1/2}) + \varepsilon(\mathbf{v}^1 + \boldsymbol{\varphi}^1 + \mathbf{w}^1) + \dots$$

- $\mathbf{v}^{k/2}$ are regular terms (with bounded derivatives).
- $\boldsymbol{\varphi}^{k/2}$ are 2D boundary layer terms exponentially decreasing with respect to $r/\sqrt{\varepsilon}$ (r is the distance to ∂S).
- $\mathbf{w}^{k/2}$ are 3D boundary layer terms exponentially decreasing with respect to r/ε . Always present (also for plates).

Energy estimate $\mathrm{E}^{\varepsilon}_{3\mathrm{D}}[\mathbf{u}^{\varepsilon} - \mathbf{Uz}] \leq b_S \varepsilon \mathrm{E}^{\varepsilon}_{2\mathrm{D}}[\mathbf{z}]$.

In this case, we obtain, $L \simeq \varepsilon^{1/2}$, $R \simeq 1$.

Koiter's estimate $\mathrm{E}^{\varepsilon}_{3\mathrm{D}}[\mathbf{u}^{\varepsilon} - \mathbf{Uz}] \leq c_S \left(\frac{\varepsilon^2}{L^2} + \frac{\varepsilon}{R}\right) \mathrm{E}^{\varepsilon}_{2\mathrm{D}}[\mathbf{z}]$ is

valid for clamped elliptic shells.

The case of plates

In this case, a complete asymptotic expansion exists, including 3D boundary layers
[Dauge & Gruais (1996-1998), Dauge, Gruais & Rössle (1999)]

Energy estimate $\mathrm{E}^{\varepsilon}_{3\mathrm{D}}[\mathbf{u}^{\varepsilon} - \mathbf{U}\mathbf{z}] \leq b_S \varepsilon \mathrm{E}^{\varepsilon}_{2\mathrm{D}}[\mathbf{z}]$.

The Koiter model splits into the 2D membrane operator acting on z_α and the bending operator acting on z_3. Asymptotic expansion of $\mathbf{z}$ without boundary layers.

$L \simeq 1$ and $1/R = 0$.

Koiter's estimate $\mathrm{E}^{\varepsilon}_{3\mathrm{D}}[\mathbf{u}^{\varepsilon} - \mathbf{U}\mathbf{z}] \leq c_S \left(\frac{\varepsilon^2}{L^2} + \frac{\varepsilon}{R}\right) \mathrm{E}^{\varepsilon}_{2\mathrm{D}}[\mathbf{z}]$ is
NOT valid for plates .

Shallow shells

1. G. Andreoiu, M. Dauge, E. Faou, CRAS (2000).
2. G. Andreoiu, E. Faou, Asymptotic analysis, (2001).

In this case, the curvature of S is of order ε.
When $\varepsilon \to 0$, the mean surface S tends to a domain of $\mathbb{R}^2$.
The Koiter model is a weak coupled system.

We have $1/R \simeq \varepsilon$ and $L \simeq 1$.

Energy estimate as for plates $\mathrm{E}^{\varepsilon}_{3\mathrm{D}}[\mathbf{u}^{\varepsilon} - \mathbf{Uz}] \leq b_S \varepsilon \mathrm{E}^{\varepsilon}_{2\mathrm{D}}[\mathbf{z}]$.

Koiter's estimate $\mathrm{E}^{\varepsilon}_{3\mathrm{D}}[\mathbf{u}^{\varepsilon} - \mathbf{Uz}] \leq C_S \left(\frac{\varepsilon^2}{L^2} + \frac{\varepsilon}{R} \right) \mathrm{E}^{\varepsilon}_{2\mathrm{D}}[\mathbf{z}]$ is

NOT valid for shallow shells.

Koiter estimate revisited

1. M. Dauge, E. Faou, *Koiter estimate revisited*, Rapport de recherche INRIA RR-5430.

New estimate, optimal in the previous three cases.

New estimate

$$\mathrm{E}^{\varepsilon}_{3\mathrm{D}}\big[\mathbf{u}-\mathbf{U}\mathbf{z}\big] \le a_S\left(\frac{\varepsilon}{\ell}+\frac{\varepsilon^2}{\mathrm{r}^2}+\frac{\varepsilon^2}{L^2}+\frac{\varepsilon^4\mathrm{D}^2}{L^6}\right)\mathrm{E}^{\varepsilon}_{2\mathrm{D}}[\mathbf{z}] + a_S\mathrm{D}^2E^{-1}\|\mathbf{f}^{\mathrm{rem}}\|^2_{\mathrm{L}^2(\Omega^\varepsilon)}.$$

- a_S is an adimensional constant,
- L is a global wave length for $\mathbf{z}$ similar to the one which Koiter used,
- ℓ is a lateral wave length for $\mathbf{z}$ (boundary layers).
- r is a constant depending on the curvature of S,
- D is a constant appearing in the 3D Korn inequalities,
- E is the Young modulus ($E=\mu(3\lambda+2\mu)/(\lambda+\mu)$)
- $\mathbf{f}^{\mathrm{rem}}=\mathbf{f}^\varepsilon-\frac{1}{2\varepsilon}\int_{-\varepsilon}^{\varepsilon}\mathbf{f}^\varepsilon(\mathrm{x}_3)\mathrm{d}\mathrm{x}_3$.
- Optimal inequality in the previous three cases.

Eigenmodes problem

The problem is more difficult.

Complete asymptotic expansion in the case of plates:

- M. Dauge, I. Djurdjevic, E. Faou, A. Roessle, *Eigenmode Asymptotics in Thin Elastic Plates* (1999)

Open problems for the other cases. Numerical investigation.

- M. Dauge, E. Faou, Z. Yosibash, *Plates and shells: Asymptotic expansions and hierarchical models*. Chapter 8, Vol I of the Encyclopedia for Computational Mechanics. (2004).

Example in the case of clamped elliptic shell:

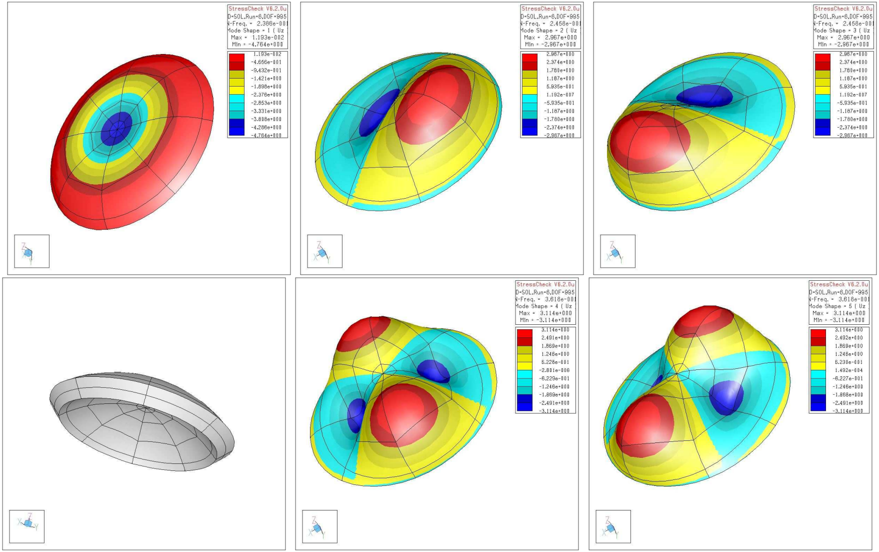
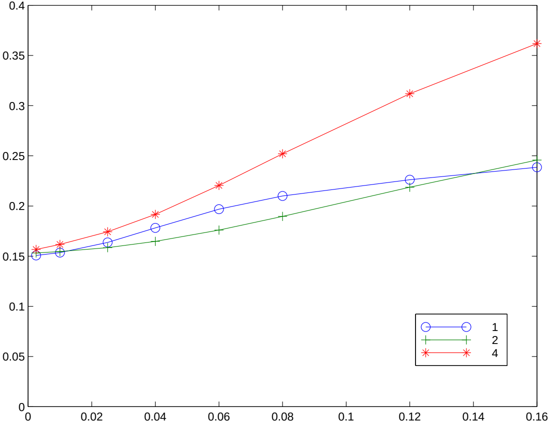


Figure: Vertical components of first 5 eigen-modes for $\varepsilon = 0.16$



No convergence towards a discrete spectrum

Problem: essential spectrum in the membrane operator

Analysis in axisymmetric situations: PhD work of Marie Beaudoin.

Numerical integration of Hamiltonian systems and molecular dynamics

Hamiltonian systems

Ordinary differential equations systems of the form

$$\begin{aligned} \dot{p} &= -\partial_q H(p,q) \\ \dot{q} &= \partial_p H(p,q)) \end{aligned}$$

$p \in \mathbb{R}^d$, $q \in \mathbb{R}^d$, $\dot{q}$ time derivative of $q(t)$.
Solution with initial values $q(0)$ and $p(0)$.

$H(p,q)$ energy function.

Example: $H(p,q) = \frac{1}{2}\sum_{k=1}^{d} p_k^2 + U(q)$ (Kinetic and potential energies) .

$$\dot{p}_k = -\nabla_k U(q) \quad \text{and} \quad \dot{q}_k = \frac{p_k}{m_k}$$

Newton's law.

Properties

We can write the system as follows, with $y = (p, q) \in \mathbb{R}^{2d}$

$$\dot{y} = J^{-1}\nabla H(y) \quad \text{where} \quad J = \begin{pmatrix} 0 & I_d \\ -I_d & 0 \end{pmatrix}$$

is the canonical symplectic matrix.

- Conservation of the Energy: $H(y(t)) = H(y(0))$.
- The flow $\varphi_t(y_0)$ is symplectic:

$$\forall\, t \geq 0, \forall\, y_0 \in \mathbb{R}^{2d} \quad \partial_{y_0}\varphi_t(y_0)^T J \partial_{y_0}\varphi_t(y_0) = J.$$

Implies the conservation of the volume $\det(\partial_{y_0}\varphi_t(y_0)) = 1$.

Important in molecular dynamics.

Numerical simulation

Numerical flow $\Phi_h(y) \simeq \varphi_h(y)$ for a small step size $h > 0$.

Example: Verlet integrator in the case where $H(p,q) = \dfrac{1}{2}\sum_{k=1}^{d} p_k^2 + U(q)$.

$(p_1, q_1) = \Phi_h(p_0, q_0)$ defined by

$$
\begin{aligned}
p_{1/2} &= p_0 - \tfrac{h}{2}\nabla_q U(q_0)\\
q_1 &= q_0 + h p_{1/2}\\
p_1 &= p_{1/2} - \tfrac{h}{2}\nabla_q U(q_1)
\end{aligned}
$$

Splitting scheme associated with the decomposition

$$H(p,q) = T(p) + U(q).$$

Symplectic scheme. $\partial_{y_0}\Phi_h(y_0)^T J \partial_{y_0}\Phi_h(y_0) = J.$

Backward error analysis

Let Φ_h be a symplectic scheme of order p, and $y_{n+1} = \Phi_h(y_n)$, $n \geq 0$.

Then y_n coincide with the solution $\tilde{y}(nh)$ of a system

$$\frac{\mathrm{d}\tilde{y}}{\mathrm{d}t}(t) = J^{-1}\nabla \tilde{H}_h(\tilde{y}(t))$$

over VERY long times $(nh \leq \exp(-1/h))$ where

$$\tilde{H}_h(y) = H(y) + \mathcal{O}(h^p)$$

$\Longrightarrow$ conservation of the energy over very long time, up to an error h^p.

[Benettin & Giorgilli (1994), Hairer & Lubich (1997), Reich (1999)]

Gaussian wave packets dynamics

1. E. Faou, C. Lubich, Computing and Visualization in Science (2006).
2. Erwan Faou and Vasile Gradinaru, Submitted.

Goal: Approximation of the Schrödinger equation.

Time-dependent Schrödinger equation in quantum MD

$$i\varepsilon \frac{\partial \psi}{\partial t} = H\psi, \qquad \psi(x,0) = \psi_0(x).$$

- Wave function $\psi = \psi(x,t)$, $x = (x_1, \dots, x_N)$ with $x_k \in \mathbb{R}^d$ ($d = 1$ or 3) and time $t \in \mathbb{R}$.
- Hamiltonian $H = T + V$ with the kinetic and potential energy operators

$$T = -\sum_{k=1}^{N} \frac{\varepsilon^2}{2m_k} \Delta_{x_k} \quad \text{and} \quad V = V(x),$$

  Particle mass: $m_k > 0$. Laplace operator Δ_{x_k}. Real potential $V(x)$.
- ε is a (small) positive number representing the scaled Planck constant.
- Preservation of the L^2 norm .

Dirac-Frenkel-McLachlan Principle

- $\mathcal{M} \subset L^2$ an approximation manifold.
- $T_u\mathcal{M}$ the tangent space at $u \in \mathcal{M}$ (the space of admissible variations).
- $t \mapsto u(t)$ solution of

$$\mathrm{Re}\,\langle \delta u, \frac{\partial u}{\partial t} - \frac{1}{i} H u \rangle = 0 \quad \text{for all} \quad \delta u \in T_u\mathcal{M}.$$

  This amounts to

$$\frac{\partial u}{\partial t} = P(u) \frac{1}{i} H u.$$

  with the orthogonal projection $P(u) : \mathcal{H} \to T_u\mathcal{M}$

- Applications: Time-dependent Hartree, Hatree-Fock, MCTDH, Gaussian wave packets, etc...

Gaussian wave packets

$\mathcal{M}$ made of functions of the form $u(x,t) = e^{i\phi(t)/\varepsilon} \prod_{k=1}^{N} \varphi_k(x_k,t)$ with

$$\varphi_k(x_k,t) = \exp\Big(\frac{i}{\varepsilon}\big(a_k(t)\,|x_k - q_k(t)|^2 + p_k(t)\cdot(x_k - q_k(t)) + c_k(t)\big)\Big).$$

Finite dimensional complex submanifold parametrized by

- $q_k = \langle\, u \,|\, x_k \,|\, u \,\rangle \in \mathbb{R}^d$ position average
- $p_k = \langle\, u \,|\, -i\varepsilon\nabla_{x_k} \,|\, u \,\rangle \in \mathbb{R}^d$ momentum average
- $a_k = \alpha_k + i\beta_k$ (with $\beta_k > 0$) complex width parameter,
- $c_k = \gamma_k + i\delta_k$ complex phase parameter, and ϕ a real phase.

[Heller (1975), Lee & Heller (1982), Coalson & Karplus (1990)]

GWP equations

$$
\begin{aligned}
\dot{q}_k &= \frac{p_k}{m_k}\\
\dot{p}_k &= -\langle\, u \,|\, \nabla_{x_k} V \,|\, u \,\rangle\\
\dot{a}_k &= -\frac{2a_k^2}{m_k} - \frac{1}{2d}\langle\, u \,|\, \Delta_{x_k} V \,|\, u \,\rangle\\
\dot{c}_k &= \frac{i\varepsilon d a_k}{m_k} + \frac{\varepsilon}{8\beta_k}\langle\, u \,|\, \Delta_{x_k} V \,|\, u \,\rangle\\
\dot{\phi} &= \sum_{k=1}^{N} \frac{|p_k|^2}{2m_k} - \langle\, u \,|\, V \,|\, u \,\rangle
\end{aligned}
$$

where $(a_k = \alpha_k + i\beta_k$ and $c_k = \gamma_k + i\delta_k)$

$$
\langle\, u \,|\, W \,|\, u \,\rangle = \int_{\mathbb{R}^N} W(x) \prod_{j=1}^{N} \exp\Big(-\frac{2}{\varepsilon}(\beta_j |x_j - q_j|^2 + \delta_j)\Big) \mathrm{d}x.
$$

This average depends only on the parameters q_j, β_j, and δ_j.

Poisson structure

- The GWP system has a Poisson structure $\dot{y} = B(y)\nabla K(y)$ where $u = \chi(y)$, $y = (q_k, p_k, \ldots)$ inherited from the symplectic structure of the Schrödinger equation.
- Conservation of the energy $K(y) = \langle\, u \,|\, H \,|\, u \,\rangle$:

$$\langle\, u \,|\, H \,|\, u \,\rangle = \|u\|^2 \sum_{k=1}^{N} \left(\frac{|p_k|^2}{2m_k} + \frac{\varepsilon d}{2m_k} \frac{\alpha_k^2 + \beta_k^2}{\beta_k} \right) + \langle\, u \,|\, V \,|\, u \,\rangle.$$

  As $\varepsilon \to 0$ and $\|u\| = 1$, the energy tends to the classical one.
- Conservation of the L^2-norm and of the linear and angular momentum.

Variational splitting

The decomposition $H = T + V$ induces the symmetric splitting scheme

$$u^{n+1} = \varphi^V_{\Delta t/2} \circ \varphi^T_{\Delta t} \circ \varphi^V_{\Delta t/2}(u^n)$$

- $u(t) = \varphi^V_t(u_0)$ is the solution of

$$\langle\, \delta u,\, i\varepsilon \dot{u} - Vu \,\rangle = 0 \quad \text{for all} \;\; \delta u \in T_u\mathcal{M}, \quad u(0) = u_0$$

- $u(t) = \varphi^T_t(u_0)$ is the solution of

$$\langle\, \delta u,\, i\varepsilon \dot{u} - Tu \,\rangle = 0 \quad \text{for all} \;\; \delta u \in T_u\mathcal{M}, \quad u(0) = u_0$$

Projection of the Strang or symmetric Trotter splitting algorithm.
[Lubich (2004)]

Tübingen's miracle

Each part of the splitting can be computed exactly!!

For the kinetic part: Logic . For the potential part: Magic .

$u_1 = \varphi^V_{\Delta t}(u_0)$, where $u_0 = \chi(q^0, p^0, a^0, c^0, \phi^0)$:

$$\left.\begin{array}{rcl} \dot{q} &=& 0 \\ \dot{p} &=& -\langle\, u \,|\, \nabla_x V \,|\, u \,\rangle \\ \dot{a} &=& -\frac{1}{2d}\langle\, u \,|\, \Delta_x V \,|\, u \,\rangle \in \mathbb{R} \\ \dot{c} &=& \dfrac{\varepsilon}{8\beta}\langle\, u \,|\, \Delta_x V \,|\, u \,\rangle \in \mathbb{R} \\ \dot{\phi} &=& -\langle\, u \,|\, V \,|\, u \,\rangle \end{array}\right\} \Longrightarrow \quad \dot{q} = 0,\ \dot{\beta} = 0,\ \dot{\delta} = 0.$$

$\langle\, u_0 \,|\, W \,|\, u_0 \,\rangle$ depends only on q^0,β^0 and δ^0

$\Longrightarrow$ **The solution is explicit** .

Properties

- **Poisson integrator** that preserves the L^2 norm, and the linear and angulum momentum.
- Order 2:

$$\big\| |u^n|^2 - |u(t^n)|^2 \big\| = O(\Delta t^2) \quad \text{but} \quad \|u^n - u(t^n)\| = O(\Delta t^2/\varepsilon).$$

- Energy conservation: if the q_k are bounded and if $\beta_k \geq c_0\varepsilon$

$$\Big| \langle\, u^n \,|\, H \,|\, u^n \,\rangle - \langle\, u^0 \,|\, H \,|\, u^0 \,\rangle \Big| \leq C\Delta t^2 \qquad \text{for} \quad n\Delta t \leq \exp(c/\Delta t)$$

where the constants are independent of Δt, and ε.

Work in progress: Hagedorn wave packets
(In collaboration with C. Lubich and V. Gradinaru)

Other results in geometric integration

Splitting methods for the linear Schrödinger equation

Schrödinger equation with periodic boundary conditions

$$i\frac{\partial u}{\partial t}(t,x) = -\Delta u(t,x) + V(x)u(t,x).$$

Splitting: $u(t) = \exp(it(\Delta - V)) \simeq \exp(it\Delta)\exp(-itV)$.

- No backward error analysis (infinite dimensional problem).
- Normal form result: perturbation of linear operators with V small.
- Part of Guillaume Dujardin's PhD work (2008)

1. G. Dujardin, E. Faou, to appear in Numerische Mathematik.
2. G. Dujardin, E. Faou, CRAS (2007).

Some results in geometric integration

- **Energy conservation for symetric methods**
  E. Faou, E. Hairer, T.-L. Pham, BIT (2004).
- **Quadratic and Hamiltonian invariants**
  P. Chartier, E. Faou, A. Murua, Numerische Mathematik (2006) .
- **Piecewise smooth Hamiltonian**
  P. Chartier, E. Faou, To appear in M2AN.
- **Application to Raman lasers**
  1. F. Castella, P. Chartier, E. Faou, CRAS (2003) 703-708.
  2. F. Castella, P. Chartier, E. Faou, D. Bayart, F. Leplingard, C. Martinelli, M2AN, (2004).
  3. F. Leplingard, C. Martinelli, S. Borne, L. Lorcy, T. Lopez, D. Bayart, F. Castella, P. Chartier, E. Faou, IEEE Photonics Technology Letters (2004).

Application to Molecular dynamics

Principle of molecular dynamics

Hamiltonian system $\dot{y} = J^{-1}\nabla H(y)$.

Energy conservation + volume conservation

$\Longrightarrow$ Preservation of the microcanonical measure.

Ergodic hypothesis: For all function f

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T f(\varphi_t(y))\mathrm{d}t = \int_{\Sigma_0} f(x)\frac{\mathrm{d}\sigma(x)}{\|\nabla H(x)\|}$$

where $\Sigma_0 = \{y \in \mathbb{R}^{2d} | H(y) = H(y_0)\}$.

Principle: simulate the left-hand side to compute the right-hand side.

Problem: hypothesis fails in general (in particular for integrable systems)

Averaging for integrable dynamics

1. E. Cancès, F. Castella, P. Chartier, E. Faou, C. Le Bris, F. Legoll, G. Turinici, Journal of Chemical Physics, 121 (2004) 10346-10355.
2. E. Cancès, F. Castella, P. Chartier, E. Faou, C. Le Bris, F. Legoll, G. Turinici, Numerische Mathematik 100 (2005) 211–232.

Idea : when the system is integrable, we can accelerate the convergence of the time average.

Application : Highly-oscillatory systems?

Shakers in molecular dynamics

Instead of considering hamiltonian system, $\dot{y} = J^{-1}\nabla H(y)$, we introduce systems of the form:

$$\dot{y} = J(t)\nabla H(y)$$

where J is a time dependent matrix.

Idea : $J(t)$ skew-symmetric $\Longrightarrow$ Energy and volume conservation.

Goal : $J(t)$ **shakes** the system to break the possible other invariants.

1. E. Faou, Journal of Chemical Physics (2006).
2. E. Faou, T. Lelièvre, *Ergodic stochastic differential equations for computing microcanonical averages.* In preparation.

Stochastic extension : we can prove the ergodicity, and the ergodicity of numerical schemes.

Work in progress with T. Lelièvre.

Future works

Hybrid methods for solving parabolic systems

Reaction-diffusion problems of the form

$$\frac{\partial u}{\partial t}(t,x) = \Delta u(t,x) + g(u(t,x))$$

Splitting schemes using the solutions of $\partial_t u = \Delta u$ and $\partial_t u = g(u)$.

Probabilistic interpretation of splitting schemes yields:

- Simpler proofs of known estimates using stochastic calculus .
- New estimates (with less regularity for the reaction part)
- New schemes (hybrid schemes)

Hybrid methods for solving parabolic systems

But...

Referee:

"This manuscript suggests a new way of analyzing splitting methods which is based on stochastic analysis. It seems to me that the proposed analysis has no advantage over the 'old' analysis."

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Hybrid methods and analysis frighten away

$\Longrightarrow$ A huge work to be done in this field!!