Time-Dependent PDEs, Conservative Numerical Approximations, and The Cayley Transform Techniques


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May 12, 2010
Outline of This Talk

- Conservative numerical approximations:
  - Cayley transform and spectral theory;
  - Cayley transform in control theory and geometric integration;
  - Cayley transform in mechanics and highly oscillatory problems in control.

- Convection-diffusion model as a simple example of coupling.

- One-to-one correspondence between continuous and discrete semigroups for this model.

- Fully discrete solution based on the Cayley transform.

- Concluding remarks.
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Any multiplication operator is a (densely defined) self-adjoint operator. Any self-adjoint operator is unitarily equivalent to a multiplication operator.
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Friedrichs (1934) who analyzed a factorization procedure for the construction of a functional space where operator spectra are most tractable;


* The core of the theory was a lifting theorem stating that under certain conditions the operator can be lifted, with control on the norm.

* To which extent the preservation of the spectra can be obtained in this case?

Courant et al (1952), Godunov (1959), Arakawa (1966), Richtmyer and Morton (1967): \textit{conservative numerical approximations to PDEs} (based on the Lagrangian mechanics);
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The construction of a Hamiltonian system starts from the definition of a Lagrangian function and the corresponding action principle underlying physical principles of conservation laws;

Pontryagin et al (1955): the maximum principle and optimal control theory (Bellman, 1957); the link between HM and LM via the Hamilton-Jacobi-Bellman equation;
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Pontryagin et al (1955): the maximum principle and optimal control theory (Bellman, 1957); the link between HM and LM via the Hamilton-Jacobi-Bellman equation;

This link appears to be fundamental in the applications of the Cayley transform.
Role of the Cayley transform

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- From the systems/control theory perspective, the role of the Cayley transform is to transform the analysis of conservative and passive scattering continuous time systems into systems with analogous properties in the discrete setting. The analogous statement holds for the inverse Cayley transform.

Hamiltonian PDEs: Bridges et al (2006, 2010), focusing on the following canonical form of equations (Hamiltonian system on a multisymplectic structure):

$$\mathbf{K} \frac{\partial \mathbf{z}}{\partial t} + \mathbf{L} \frac{\partial \mathbf{z}}{\partial x} = \nabla_{\mathbf{z}} S(\mathbf{z}),$$

(1)

in which many wave propagation problems, including some conservation law systems, can be cast ($\mathbf{K}$ and $\mathbf{L}$ are constant skew-symmetric matrices).

Some of interesting points regarding symplectic integrators were raised by W. Hoover and can be found at

http://williamhoover.info/nonequilibrium.html
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Noether theorem and conservation laws

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- In applications to PDEs:
  - How does one define the symmetries?
  - How does one calculate the symmetries?
  - What does one do with the symmetries?
The discrete analogue of Noether’s theorem is applicable to equations with known variational, Hamiltonian or multisymplectic structure, but in most interesting problems we have to deal with
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- Summary of the results for the Noether-type theorems for difference equations: Dorodnitsyn (ANM, 2001; and with Budd, 2001) - initiation of lattice transformations (the lattice was no longer fixed and nontransformable).
In dealing with SM systems whose configuration space is a differentiable manifold represented by a Lie group, we can lift the equation to a space of fields with values in skew-symmetric matrices by using the Cayley transform, 

\[ y_n \rightarrow \sigma_n \rightarrow \sigma_{n+1} \rightarrow y_{n+1}, \]

\[ y_{n+1} = e^{\sigma_{n+1}} y_n \] (Iserles, 1999);
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Any differential equation evolving on a Lie group $G$ in $t$ ($t \geq t_0$) can be presented via the Lie algebra of $G$ (denoted by $g$) such that
\[
Y' = A(t, Y)Y, \quad t \geq t_0, \quad Y(t_0) = Y_0, \\
A : [t_0, \infty) \times G \rightarrow g, \quad Y_0 \in G. \quad (3)
\]
Dealing with the exponentials: Cayley transform

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\]

Iserles, Norsett (1999), Budd, Iserles (1999) demonstrated how Lie-group solvers for the above model can be constructed by a direct manipulation of the push-forward equation based on (a) Magnus expansion (1954), (b) Fer expansion (1958).
After spatial discretization:

\[
\frac{\partial u}{\partial t} = Au + b, \quad u(0) = u_0. \tag{5}
\]

Choices are:

- Runge-Kutta or multistep methods (the method of lines);

\[
u(t) = \exp(At)(u_0 + A^{-1}b) - A^{-1}b, \tag{6}\]

\[
\exp(At)v = \frac{1}{2\pi i} \int_{\Gamma} e^{zt}f(z)dz, \quad f(z) = (zI - A)^{-1}v. \tag{7}\]
Cayley transform in numerical integration and mechanics

- CT for geometric integration of ODEs (Iserles, 1999; FCM, 2001);
- Cayley-based quadratures (Marthinsen and Owren, 2001);
- CT-based technique for micromagnetics (Krishnaprasad and Tan, 2001; Landau-Lifshitz-Gilbert model: d’Aquino et al, 2005);

The CT and the CT kinematic relationships - an important tool for the analysis of N-dimensional orientations and rotations (Bottema and Roth, 1979; Sinclair and Hurtado, 2005);

The general motion of an N-dimensional body as the pure rotation of an (N+1)-dimensional body. To represent the three-dimensional rotation group by using the Cayley transform.
Zhong and Marsden (1988) - approximate symplectic algorithms cannot preserve energy for nonintegrable systems;
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* Approach the problem with a nonlinear configuration space from a **global perspective**: if the configuration manifold is open in a larger linear space, replace the update dictated by the structure of the configuration manifold with the additive update of the larger linear group.
* The Cayley transform can be used directly in place of the exponential map and it can be computed explicitly by using the von Neumann series.
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Re-emphasizing the space-time view and using the L mechanics, Marsden, Patrick, and Shkoller (1998) applied Veselov variational discretizations of the Euler-Lagrange equation;
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Kane, Marsden, Ortiz (JMP, 1999) demonstrated that variational integrators are symplectic, hence providing a link to the literature on variational methodologies for conservation laws.

Cayley transform is a natural tool in control theory (Arov and Nudelman, 1996) as conservation and time-flow invertibility are intrinsically connected, in particular for boundary control systems [Weiss, Staffans, Tucsnak (2001); Staffans (2005)].

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CT as a tool for constructing the unitary space-time modulation in signal processing (Jing and Hassibi, 2003); Guo and Zwart (2006);
Consider

\[- \epsilon \Delta u + u_x = f.\] (8)
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\[-\epsilon \Delta u + u_x = f.\]  \hspace{1cm} (11)

Apply FEM on a bounded polygonal domain:

\[
\int_\Omega (\epsilon \nabla u_h \cdot \nabla v + (u_h)_x v) \, dx = \int_\Omega f v \, dx, \quad v \in \mathcal{T}. \hspace{1cm} (12)
\]
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\]

Large Peclet numbers \((\epsilon/h \ll 1)\) - large MP-violating oscillations.
Multiple spatial scales and convection-diffusion problems

Consider

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SUPG with elementwise stabilization terms:

\[ \int_{\Omega} (\epsilon \nabla u_h \cdot \nabla v + (u_h)_x v) dx - \]

\[ \sum_{\Delta} \tau_{\Delta} \int_{\Delta} (-\epsilon \Delta u_h + (u_h)_x - f)(-\epsilon \Delta v - v_x) dx = \int_{\Omega} fv dx \]  \hspace{1cm} (19)

\( C_{\text{coerciveness}} \ll C_{\text{continuity}} \implies \text{noncoercive at the discrete level.} \)
Drift and diffusion intrinsically coupled via $\epsilon$. 
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- coupled nonlinear thermo-elasticity equations: (Matus, RM, Wang, 2004);
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Coupled dynamic problems are the rule rather than an exception in mathematics and its applications.
Find such a continuous function \( u(\cdot, t) : [0, T_0) \rightarrow E \)
\( \forall \ 0 \leq t < T_0 \) which is continuously differentiable
\( \forall \ 0 \leq t < T_0, u(\cdot, t) \in D(\mathcal{L}) \ \forall \ 0 < t < T_0, \) and which satisfies the equation

\[
\frac{\partial u}{\partial t} = \mathcal{L} u + f, \quad \mathcal{L} u = \tilde{\beta} \frac{\partial u}{\partial x} + \mu \frac{\partial^2 u}{\partial x^2} + \tilde{\alpha} u, \quad (20)
\]

with the initial condition and boundary conditions

\[
u(x, 0) = u_0(x), \quad u(d_0, t) = u(d, t) = 0. \quad (21)\]
The model describes a rich dynamics subject to the topological structure of $\mathcal{L}$. This model provides an example of a multi-physics problem coupling several physical phenomena. In particular, the model is used

- to describe the evolution of the concentration of a contaminant dropped into fluid running in a pipe;
- in the electro-magnetic theory;
- in fluid dynamics as a simplified model for fluid flow described by the Navier-Stokes system;
- as a simplified version of the drift-diffusion model in semiconductor modelling;
- in biological systems,
- and in many other areas of applications.
A special case of that model, \(-\epsilon \Delta u + u_x = f\), is part of a bigger picture

\[(\epsilon A + C)u = f,\]  \hspace{1cm} (22)

where \(A\) is symmetric second-order elliptic operator, and \(C\) is a skew-symmetric first-order differential operator, \(\epsilon > 0\). For time-dependent problems, non-trivial additional difficulties arise.
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The nonstationary counterpart of (23) with \textbf{non-self-adjoint} spatial operator is a natural candidate for applying the Cayley transform technique.
Domain decomposition is an important tool for the development of numerical algorithms parallelisable in space;
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Conventional time marching algorithms used widely for mathematical models based on time-dependent PDEs are difficult to parallelise;
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Conventional time marching algorithms used widely for mathematical models based on time-dependent PDEs are difficult to parallelise;

However, if the idea of time stepping is developed on the basis of the Cayley transform technique the parallelisation in time is natural as long as one needs to calculate the solution at different moments of times.
For the homogeneous model

\[
\frac{\partial u}{\partial t} = \mathcal{L}u, 
\]  

(24)

solution (even in a much more general situation) can be given in the form of the Dunford-Cauchy integral

\[
u(t) = \frac{1}{2\pi i} \int_{\Gamma} e^{-zt}(zI - \mathcal{L}^+)^{-1}u_0 \, dz = \frac{1}{2\pi i} \int_{\Gamma} e^{-zt}\hat{u}(z) \, dz,
\]

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where \( \hat{u} \) denotes the resolvent of the operator, that is the solution to

\[ (zI - \mathcal{L}^+)\hat{u}(z) = u_0. \]
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where \( \hat{u} \) denotes the resolvent of the operator, that is the solution to

\[
(zI - \mathcal{L}^+)\hat{u}(z) = u_0. \tag{32}\]

The integration path depends decisively on the geometric properties of the spectrum and the behaviour of the resolvent.
A positive operator $\mathcal{L}^+$ is called strongly positive if its spectral angle satisfies the inequality

$$\varphi(\mathcal{L}^+) < \pi/2.$$  \hspace{1cm} (33)
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The integral,

$$f(\mathcal{L}^+) = \frac{1}{2\pi i} \int_{\Gamma} f(z)(zI - \mathcal{L}^+)^{-1} \, dz,$$  \hfill (37)

converges in the operator norm and defines a bounded linear operator $f(\mathcal{L}^+)$,
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converges in the operator norm and defines a bounded linear operator $f(\mathcal{L}^+)$,

then the domain $D^\sigma \equiv D((\mathcal{L}^+)^\sigma)$ of the operator $(\mathcal{L}^+)^\sigma$ becomes a Banach space with the norm

$$\|u\|_{D^\sigma} \equiv \|(\mathcal{L}^+)^\sigma u\|_E.$$  \hspace{1cm} (41)
∀ \( u_0 \in E \) the CDA problem has at most one solution and such a solution can be represented in the following form

\[
u(\cdot, t) = T(t)u_0(\cdot) + \int_0^t T(t - s)f(\cdot, s)ds,
\]

where \( \{T(t)\}_{t \geq 0} \) is the analytic semigroup with the generator \( \mathcal{L} \).
The CT for Non-homogeneous CDA Problems

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where \( \{T(t)\}_{t \geq 0} \) is the analytic semigroup with the generator \( \mathcal{L} \).

The continuous semigroup \( \{T(t)\}_{t \geq 0} \) and a discrete semigroup \( \{T^n_\gamma\}_{n \geq 0} \) are intrinsically connected by the solution of the following discrete initial value problem (Arov et al)

\[
y^{n+1}_\gamma = T^n_\gamma y^n_\gamma, \ n = 0, 1, ..., \ y^0_\gamma = u_0.
\]
Further details are found in
http://www.m2netlab.wlu.ca/research/publications/EP-8-abstract.html
Remark I: on parallelization of BVPs solution

The following procedure is parallelizable in a straightforward manner:

- Set $k=0$ and compute
  \[
  F(\psi, \tilde{y}_0) = -\mu(\tilde{y}_0)'' - \tilde{\beta}(\tilde{y}_0)' - [\tilde{\alpha} + \gamma]\tilde{y}_0;
  \]

- Find the values $F(\psi_j, \tilde{y}_0)$, $j=1,\ldots,N$ (recall that $\tilde{y}^k_\gamma(\psi_0) = \tilde{y}^k_\gamma(\psi_n) = 0$);

- Using polynomial representations of $\tilde{y}^1_\gamma$ find the general form of
  $(\tilde{y}^1_\gamma(\psi))'$ and $(\tilde{y}^1_\gamma(\psi))''$ in terms of $\psi$;

- the SLAE wrt $(n-1)$ unknowns $a^{(n)}_0, \ldots, a^{(n)}_{n-2}$:
  \[
  \mu(\tilde{y}_1)' + \tilde{\beta}(\tilde{y}_1)'(\psi_j) + [\tilde{\alpha} + \gamma]\tilde{y}_1(\psi_j) = F(\psi_j, \tilde{y}_0), j = 1, \ldots, N
  \]

$\gamma$ as a parameter to speed up the convergence.
Remark II: on speeding up the convergence

If $\mathcal{L}^+$ is a strongly $P$-positive densely defined closed operator such that its spectrum is within parabola $\Gamma$, then

$$u_N(t) = \sum_{k=-N}^{N} \alpha_k e^{-z_k t} \hat{u}(z_k). \quad (46)$$

Collocation points and $\alpha_i$ can be analogous as described by Gavrilyuk, Hackbusch, and Khoromski (2002). After computing resolvents:

$$(z_j - \mathcal{L}^+) \hat{u}_{\Delta x}(z_j) = P_{\Delta x} u_0, \quad (47)$$

the fully discrete approximation (with an additional term in NH case) is

$$u_{N,\Delta x}(t) = \sum_{j=-N}^{N} \alpha_j \hat{u}_{\Delta x}(z_j) \exp(-z_j t). \quad (48)$$

Sheen, Sloan, Thomee (2003); Gavrilyuk, Makarov (2005).
Remark III: on H-Matrix Approximations

- Note further that the resolvents can be approximated with the $\mathcal{H}$-matrix arithmetics.

- If $M_j$ is the $\mathcal{H}$-matrix approximation of the resolvent, we have the following representation Hackbusch et al 2002

$$ u_{N,\mathcal{H}} = \sum_{j=-N}^{N} \alpha_j e^{-z_j t} M_j \left( u_0 + \int_0^t e^{z_j s} f(s) ds \right) $$

(49)

- The computational cost of such $\mathcal{H}$-matrix approximations, effective in data-sparse cases, is close to linear (with the linear-logarithmic theoretical estimate, Hackbusch 2000).

- The rest of the procedure remains the same as described above.
Concluding Remarks

- An alternative approach to constructing efficient time-stepping algorithms.
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The technique is part of geometric integration tools (in a sense that the integration path decisively depends on geometric properties of the spectrum and the behaviour of the resolvent) that provide numerical solutions, retaining qualitative properties of the differential systems.
Concluding Remarks

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  - The technique is part of geometric integration tools (in a sense that the integration path decisively depends on geometric properties of the spectrum and the behaviour of the resolvent) that provide numerical solutions, retaining qualitative properties of the differential systems.
  - Since the approach leads to formulae that do not require iterations in time, a parallelisation becomes natural as soon as the time marching is required.
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  - Since the approach leads to formulae that do not require iterations in time, a parallelisation becomes natural as soon as the time marching is required.

- The approach with its recent extensions is a potentially powerful tool in dealing with coupled mathematical models based on evolutionary PDEs.
Future applications of the Cayley Transform

Different aspects of this and related topics could not have been possible without collaborations with:

- Tony Roberts (Australia),
- Ivan Gavrilyuk (Germany),
- Lok Lew Yan Voon (USA),
- Morten Willatzen (Denmark),
- Benny Lassen (Denmark)

Further details on this and other projects of our group can be found at http://www.m2netlab.wlu.ca

Thank you.