Exponential Integrators using Matrix Functions: Krylov Subspace Methods and Chebyshev Expansion approximations

The HPC Approach

México, February 2018

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Outline

- Exponential Integrators
- Brief Introduction: Chebyshev expansion for matrix functions
- Brief Introduction: Krylov subspace techniques
- HPC Approach:
    - Relevance and importance of an HPC approach
    - Parallelisation strategy
- Outlook

Exponential Integrators

Matrix functions

The problem

- Consider a problem of the type

$$\frac{d\mathbf{w}(t)}{dt} = \mathbf{A}\mathbf{w}(t),\ t \in [0, T]$$

$$\mathbf{w}(0) = \mathbf{v},\ \text{initial condition}$$

- Its analytic solution is $\mathbf{w}(t) = e^{t\mathbf{A}}\mathbf{v}$

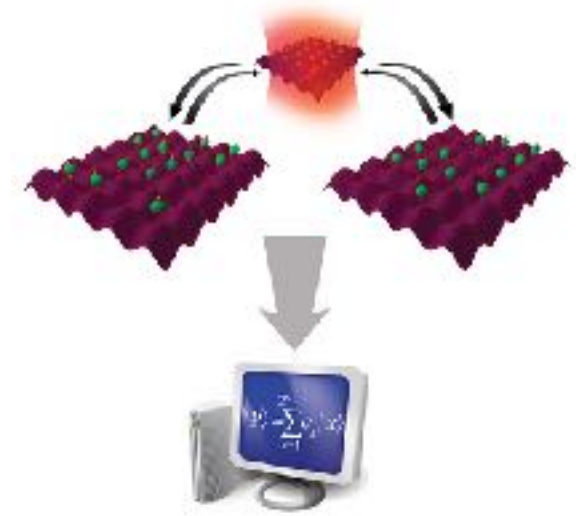
- Things to consider:

    - $\mathbf{A}$ is a matrix

    - The exponential of the matrix is not really required, but merely it's **action** on the vector $\mathbf{v}$

R. B. Sidje, ACM Trans. Math. Softw. 24, 130 (1998).

Exponential Integrators



- Mathematical models of many physical, biological and economic processes systems of linear, constant-coefficient ordinary differential equations

- Growth of microorganisms, population, decay of radiation, control engineering, signal processing…

- More advanced: MHD (magnetohydrodynamics), quantum many-body problems, reaction-advection-diffusion equations…

Moler, C. Van Loan, C. SIAM Rev. 45, 1 (2003).

Numerical approach

- The idea to use exponential functions for the matrix is **not new**
  - Was considered impractical…
- The development of Krylov subspace techniques to the **action** of the matrix exponential substantially changed the landscape
- Different types of solution evaluation for matrix exponentials:
  - ODE methods: numerical integration
  - Polynomial methods
  - Matrix decomposition methods

Moler, C. Van Loan, C. SIAM Rev. 45, 1 (2003).

Hochbruck, M. Lubich, C. Selhofer, H. SIAM J. Sci. Comp. 19, 5 (1998).

Numerical approach

- We're interested in the case where $\mathbf{A}$ is **large** and **sparse**
- A *sole* implementation may not be reliable for *all* types of problems
- Chebyshev expansion approach
- The technique of Krylov subspaces has been proven to be very efficient for **many** classes of problems
- Convergence is faster than applying the solution to linear systems in both techniques

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Take-home message #1:
There's a big number of problems in science and engineering that can be tackled using exponential integrators and matrix functions

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Polynomial approximation: Chebyshev expansion

A brief introduction

Definition

- We intend to employ a polynomial expansion as an approximation

- Let us start with a definition of the matrix exponential by convergent power series:

$$e^{t\mathbf{A}} = \mathbf{I} + t\mathbf{A} + \frac{t^2\mathbf{A}^2}{2!} + \dots$$

- An effective computation of the **action** of this operator on a vector is the main topic of this talk

Moler, C. Van Loan, C. SIAM Rev. 45, 1 (2003).

Chebyshev expansion

- We intend to employ a **good** converging polynomial expansion
- Explicit computation of $e^{\mathbf{A}t}$ **has** to be avoided
- **Key component**: Efficient matrix-vector product operations
- **Upside**: Efficient parallelisation and vectorisation, extremely simple approach
- **Downside**: Requires computation of two eigenvalues, not so versatile

Chebyshev polynomials

- The polynomials are defined by a three-term recursion relationship in the interval $x \in [-1, 1]$:

$$T_0(x) = 1$$

$$T_1(x) = x$$

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$$

- $T_n(x)$ constitutes an orthogonal basis, therefore one can write:

$$f(x) = \sum_{n=0}^{\infty} b_n T_n(x) \approx \sum_{n=0}^{N} b_n T_n(x)$$

- with $b_n = \frac{2 - \delta_n}{\pi} \int_{-1}^{1} \frac{f(y)T_n(y)}{\sqrt{1 - y^2}} dy$

Bessel coefficients for the particular case of the exponential function

Sharon, N. Shkolniski, Y. arXiv preprint arXiv:1507.03917 (2016)

Kosloff, R. Annu. Rev. Phys. Chem. 45, 145-78. (1994)

Chebyshev polynomials

- We're interested in applying the approximation to the action of the operator on a vector
- First step: Find the extremal eigenvalues of $\mathbf{A}$, more on this later

$$\lambda_{min} \quad \lambda_{max}$$

- Second step: Rescale operator such that it's spectrum is bounded by $[-1, 1]$

$$\mathbf{A}^{'} = 2\frac{\mathbf{A} - \lambda_{min}\mathbf{I}}{\lambda_{max} - \lambda_{min}} - \mathbf{I}$$

- Third step: Use the Chebyshev recursion relation

$$f(t\mathbf{A}')\mathbf{v} = e^{t\mathbf{A}'}\mathbf{v} \approx \sum_{n=0}^{N} b_n T_n(t\mathbf{A}')\mathbf{v}$$

- The recursion can be truncated up to a desired tolerance

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Chebyshev recursion relation

- The recursion relation

$$f(t\mathbf{A}')\mathbf{v} = e^{t\mathbf{A}'}\mathbf{v} \approx \sum_{n=0}^{N} b_n T_n(t\mathbf{A}')\mathbf{v}$$

- Goes as follows:

$$\phi_0 = \mathbf{v}$$
$$\phi_1 = t\mathbf{A}'\mathbf{v}$$
$$\phi_{n+1} = 2t\mathbf{A}'\phi_n - \phi_{n-1}$$

- Then:

$$f(t\mathbf{A}')\mathbf{v} \approx \sum_{n=0}^{N} b_n \phi_n$$

- Until desired tolerance

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Chebyshev polynomials

- Why do we choose the Chebyshev polynomials as basis set? Why not another polynomial set?

- Because of the asymptotic property of the Bessel function!

    - When the order n of the polynomial becomes larger than the argument, the function decays **exponentially** fast

    - This means that in order to obtain a good approximation, an exponentially decreasing amount of terms are required in the expansion as a function of the argument (related to t, λ_{min} and λ_{max})

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Take-home message #2:
The Chebyshev expansion approach provides a numerically stable and scalable approach at the cost of some restrictions of the problem

Krylov subspace techniques to evaluate the solution

A brief introduction

Krylov subspace techniques

- We intend to employ a combination of a Krylov subspace technique and other known methods for matrix exponential
- Explicit computation of $e^{\mathbf{A}t}$ **has** to be avoided
- **Key component**: Efficient matrix-vector product operations
- **Upside**: Extremely versatile
- **Downside**: Storage of the subspace for large problems, “time scales”

Main idea

- Building a Krylov subspace of dimension m

$$\mathcal{K}_m = \mathrm{span}\{v, \mathbf{A}v, \mathbf{A}^2 v, \ldots, \mathbf{A}^{m-1} v\}$$

- The idea is to approximate the solution to the problem by an element of $\mathcal{K}_m$

- In order to manipulate the subspace, it's convenient to generate an orthonormal basis

$$V_m = [v_1, v_2, \ldots, v_m] \qquad v_1 = v/||v||_2$$

- This can be achieved with the **Arnoldi algorithm**

Gallopoulos, E. Saad, Y. ICS. 89', 17—28 (1989).

Moler, C. Van Loan, C. SIAM Rev. 45, 1 (2003).

Algorithm: Arnoldi

1. *Initialize:* Compute $v_1 = v/\|v\|_2$.
2. *Iterate:* Do $j = 1, 2, ..., m$
   (a) Compute $w := Av_j$
   (b) Do $i = 1, 2, \ldots, j$
      i. Compute $h_{i,j} := (w, v_i)$
      ii. Compute $w := w - h_{i,j}v_i$
   (c) Compute $h_{j+1,j} := \|w\|_2$ and $v_{j+1} := w/h_{j+1,j}$.

- Step 2-b is a modified Gram-Schmidt process.
- **Lanczos** can be applied for the case of symmetric matrices

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Krylov subspace techniques

- The Arnoldi procedure produces a basis V_m of $\mathcal{K}_m$ and an upper Hesseberg matrix $\mathbf{H}_m$ of dimension $m \text{ x } m$ with coefficients h_{ij}

- We start by the relation given by

$$\mathbf{A}V_m = V_m\mathbf{H}_m + h_{m+1,m}v_{m+1}e_m^T$$

- Where v_{m+1} satisfies $V_m^T v_{m+1} = 0$ and $e_m \in I_m$

- From which we obtain

$$\mathbf{H}_m = V_m^T \mathbf{A} V_m$$

- Therefore, $\mathbf{H}_m$ is the projection of the linear transformation $\mathbf{A}$ onto the Krylov subspace $\mathcal{K}_m$ with respect to the basis V_m

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Krylov subspace techniques

- Given that $\mathbf{H}_m$ is a projection of the linear operator, an approximation can be made such that

$$e^{t\mathbf{A}}v \approx ||v||_2 V_m e^{t\mathbf{H}_m} e_1$$

- The approximation is **exact** when the dimension of the Krylov subspace is equal to the dimension of the linear transformation

- Error

$$||e^{t\mathbf{A}}v - ||v||_2 V_m e^{t\mathbf{H}_m} e_1|| \leq 2||v||_2 \frac{(t||A||_2)^m e^{t||A||_2}}{m!}$$

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Krylov subspace techniques

- With this approach:
  - A **large sparse** matrix problem is approximated by a **small dense** matrix problem
- There are several methods to evaluate the small dense matrix exponential
  - Series methods, ODE methods, diagonalisation, matrix decomposition methods…
  - Padè methods
- This method can be used to compute λ_{min} and λ_{max} for the Chebyshev approach, very effective

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Take-home message #3:
Krylov subspace methods to evaluate the solution provides a more versatile and less restricted approach, at the expense of higher computational cost and memory consumption

HPC Approach

Relevance and importance

- A platform for numerical calculations
  - Important for current research
- Undertake simulations efficiently
- Quantum physics, CFD, finite-element methods…
- Establish an instance where HPC approach has been used recently in scientific research

Parallelisation strategy

$$y = \mathbf{A}x$$

- The linear operator is **sparse** (low density) and **huge** (big dimension, i.e, large amount of degrees of freedom

- Approach:
  - **Distribute the operator among processing elements**

Take-home message #4:
Your numerical evaluation of the exponential integrator using matrix functions is only going to be **as good as** your implementation of the sparse matrix-vector product

Outlook

- Two different approximation methods to target the solutions to matrix exponentials, which can be interpreted analytically as solutions to a particular set of differential equations
- We will discuss the practical approach using techniques, practices and libraries from the HPC perspective next session…

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Thank you!