

### To be filled in

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### **Preface**

To be filled in!

## Acknowledgment

To be filled in.

## **Summary and Conclusions**

To be filled in!

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### Introduction

Skrive litt om problemet, layouten og slikt.
!!!!!!!!!!!!!!!cite rapport og SLM !!!!!!!!!!!!

The equation

$$\dot{u}(t) = Au(t) + F(t)$$

$$u(0) = u_0$$
(1.1)

often makes an appearance when solving partial differential equations with numerical methods. The author has earlier observed how the heat equation, discretized with finite difference methods to be on the form of equation (1.1) can be solved with the use of the Krylov projection method(KPM) [1]. This note will continue on the same track, with more focus on the wave equation, and energy preservation. It will also feature a comparison between Symplectic Lanzcos method(SLM) [3] and KPM. SLM is a projection technique that only works on Hamiltonian matrices. Due to this, SLM (claim to) preserve energy better than KPM.

!!!!!!!!!!MÅ cite forsjkellig når jeg vil/anbefaler å lese hele, og når jeg anbefaler å lese deler av det!!!!!!!

### **Explonation**

There will here be a short explanation of all solvers, constants, outdata and expressions used in this text. Matlab notation is used where applicable. Fell free to go straight to next chapter, and use this as a reference later in the note.

### 2.1 Projection methods

As mentioned earlier, two projection methods will be presented, KPM and SLM. They are very similar in nature, with the only difference being the orthogonalisation method. KPM uses Arnoldi's algorithm, given in Algorithm 1, and SLM uses the symplectic Lanczos method, given in Algorithm 2. The framework is given in Algorithm 3.

Note that n given to Algorithm 2 is half the size of n given to Algorithm 1, due to the way the orthogonalisation is done.

The approximated solution, found by either SLM or KPM, will be denoted as  $u_n$ , where n the same as above.

If the solution is obtained without the use of an orthogonalisation, it will be denoted with DM for direct method.

#### Algorithm 1 Arnoldi's algorithm[7]

```
Start with A \in \mathbb{R}^{m \times m}, v \in \mathbb{R}^m, n \in \mathbb{N} and e \in \mathbb{R}.

v_1 = v/\|v\|_2

for j = 1, 2, \cdots, n do

Compute h_{i,j} = v_i A v_j, v_i for i = 1, 2, \cdots, j

Compute w_j = A v_j - \sum_{i=1}^j h_{i,j} v_i

h_{j+1,j} = \|w_j\|_2

if h_{j+1,j} < e then

STOP

end if

v_{j+1} = w_j/h_{j+1,j}

end for

Return H, V, v_{n+1}, h_{n+1,n}.
```

#### Algorithm 2 Symplectic Lanczos method [3], with reortogonalization from [2].

```
Start with a Hamiltonian matrix A \in \mathbb{R}^{2m \times 2m}, \tilde{v}_1 \in \mathbb{R}^{2m}, n \in \mathbb{N}
v_0 = 0 \in \mathbb{R}^{2m}
\xi_1 = \|\tilde{v}_1\|_2
v_1 = \frac{1}{\xi_1} \tilde{v}_1
for j = 1, 2, \dots, n do
      v = Av_i
     \delta_{j} = v_{j}^{\dagger}
\tilde{w} = v - \delta_{j} v_{j}

\kappa_j = v_j^{\mathsf{T}} J v

     w_j = \frac{1}{\kappa_i} \tilde{w}_j
      w = Aw^{j}
     \tilde{V}_{j-1} = [v_1, v_2, \cdots, v_{j-1}, w_1, w_2, \cdots, w_{j-1}]
     w_{j} = w_{j} + \tilde{V}_{j-1}J_{j-1}\tilde{V}_{j-1}^{\top}J^{m}w_{j}
     \beta = -w_i^{\mathsf{T}} J w
     \tilde{v}_{j+1} = w - \xi_j v_{j-1} - \beta_j v_j + \delta_j v_j
     \xi_{j+1} = \|\tilde{v}_{j+1}\|_2
v_{j+1} = \frac{1}{\xi_{j+1}} \tilde{v}_{j+1}
     \begin{split} \tilde{V}_j &= [v_1, v_2, \cdots, v_j, w_1, w_2, \cdots, w_j] \\ v_{j+1} &= v_{j+1} + \tilde{V}_j J_j \tilde{V}_j^\top J_m v_{j+1} \end{split}
V = [v_1, v_2, \dots, v_n, w_1, w_2, \dots, w_n]
H = \left[ \operatorname{diag}([\delta_j]_{j=1}^n) \quad \operatorname{tridiag}([\xi]_{j=2}^n, [\beta]_{j=1}^n, [\xi]_{j=2}^n) \right]
Return H, V, v_{n+1}, \xi_{n+1}.
```

#### Algorithm 3 The Krylov projection method with restart[1]

```
Start with A \in \mathbb{R}^{m \times m}, f(t), v \in \mathbb{R}^m, n \in \mathbb{N}, a boolean value restart, an algorithm alg, \epsilon \in \mathbb{R},
and i = 0.
Compute [V_n, H_n, h_{n+1,n}^i, v_{n+1}] = alg(A, v, n)
Solve z'_{i}(t) = H_{n}z_{i}(t) + f(t) ||v||_{2}e_{1} for z_{i}(t)
u_n(t) \leftarrow V_n z_i(t)
\delta = h_{n+1,n}
if restart == 1 then
   while \epsilon < \delta do
       i \leftarrow i + 1
      Compute [V_n, H_n, h_{n+1,n}^i, v_{n+1}] = alg(A, v_{n+1}, n)
      Solve z'_i(t) = H_n z_i(t) + h_{n+1,n}^{i-1} e_n^{\top} z_{i-1}(t) for z_i(t)
       u_n(t) \leftarrow u_n(t) + V_n z_i(t)
       \delta = \max(u_n(t) - V_n z_i(t))
   end while
end if
Return u_n.
```

#### 2.2 Zero initial condition

For both KPM and SLM it is important that the initial conditions are zero. Equation (1.1) can be transformed so that it has zero initial conditions in the following way:

$$\hat{u}(t) = u(t) - u_0$$

The original equation can then be written as

$$\hat{u}(t) = A\hat{u}(t) + Au_0 + F(t)$$

$$\hat{u}(0) = 0 \qquad (2.1)$$

$$u(t) = \hat{u} + u_0$$

All test problems with a non-zero initial condition will be transformed in this way.

#### 2.3 Discretization

!!!!!!!!!Figurer over simulert tid må være med ekte simulert tid fra 0 til 1(tror dette er fikset!, trenger bare nye bilder)!!!!!!!!!!!!!!

The number of points in each spacial direction is m, this gives makes the step size  $h_s = 1/m$ . The number of steps in time is k, this makes the step size  $h_t = 1/k$ .

Let the matrix *I* be the identity matrix of appropriate size, and let

$$J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} \tag{2.2}$$

of appropriate size.

Equation (1.1) can be the result of the discretization of several equation. Since SLM needs a Hamiltonian matrix, this is the main focus. One of the two implemented matrices is the discretization of the 2 dimensional wave equation,

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + f(t, x, y). \tag{2.3}$$

This can be discretized to be on the form of equation (1.1), with the matrix

$$\tilde{A} = \frac{2}{h_s^2} \text{ gallery('poisson', } m-2)$$

$$A = \begin{bmatrix} 0 & I \\ -\tilde{A} & 0 \end{bmatrix}$$
(2.4)

The matrix  $\tilde{A}$  is also known as the five-point stencil. This matrix will be referred to as wave when used. The second implemented matrix is a random Hamiltonian matrix, given by

$$\hat{A} = \text{rand}(2(m-2)^2)A = \frac{1}{2}J(\hat{A} + \hat{A}^{\top} + m^2I). \tag{2.5}$$

Since we are interested in comparing the different projection methods to each other, the matrix will be saved and reused when necessary. This matrix will be referred to as semirandom. The

part  $m^2I$  is added to make JA diagonally dominant, there would be no way of knowing if any of the methods would converge without this part.

These two matrices also has some test problems that satisfies the condition: u(t,0,y) = u(t,1,y) = u(t,x,0) = u(t,x,1) = 0.

In the case when the energy is constant and wave is used, the test problem is

$$u(t, x, y) = \sin(\pi x)\sin(\pi y)\cos(\sqrt{2\pi}t)$$

$$u_0 = \sin(\pi x)\sin(\pi y)$$

$$f(t, x, y) = 0,$$
(2.6)

and

$$u(t, x, y) = \text{unknown}$$

$$u_0 = \text{rand}(2(m-2)^2, 1)$$

$$f(t, x, y) = 0$$
(2.7)

for semirandom. This test problem is kept with the same conditions as A.

The source term f(t, x, y) is chosen to be zero because it is easier to work with a constant energy. Some problems with non-constant energy will be presented later.

### 2.4 Lingo

There will here be a short explanation of the labels on the figures you will see later.

iterations number of restarts performed by Arnoldi or symplectic lanczos method.
time elapsed when solving the problem (y-axis)
error1 Difference in error between analytical solution, and estimated solution.
energy2 Difference between the largest and smallest energy during the simulated time.

Table 2.1: Explanation of the labels on the y-axis.

  $\begin{array}{ll} m & \text{number of point in each spacial direction} \\ n & \text{restart variable} \\ k & \text{number of points in time} \\ t & \text{simulated time} \\ \text{restart} & \text{a boolean value. If restart == 1, Arnoldi or} \\ & \text{symplectic Lanczos method will restart.} \\ \epsilon & \text{if restart is true, restarting will} \\ & \text{commence until the change in the solution} \\ & \text{is less than } \epsilon \end{array}$ 

Table 2.2: Explanation of the labels on the x-axis.

!!!!!!!!!Fyll inn etterhvert som du trenger det!!!!!!!!!!!!!

### Compare time integration methods

!!!!!!!!!!!!Endre *y*( *u* eller *U*) til noe annet!!!!!!!!!!!!!

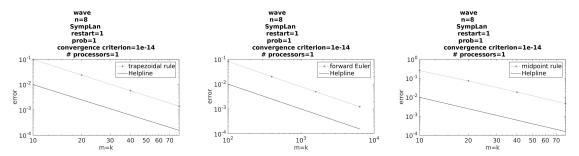
This section will be concerned with comparing the integrators. How well they estimate the error and energy will be the primary concern.

The relevant integrators are trapezoidal rule, forward euler, and midpoint rule. The definition, and the iteration scheme, of the different methods are given in the table below.

Convergence of the different methods are shown in figure 3.1

Trapezoidal rule [4] 
$$y_{i+1} = y_i + h_t f\left(\frac{1}{2}(t_n + t_{n+1}), \frac{1}{2}(y_n + y_{n+1})\right)$$
  $y_{i+1} = (I - \frac{Ah_t}{2}) \setminus \left(y_i + \frac{h_t}{2}\left(Ay_i + (F_{i+1} + F_i)\right)\right)$   
Forward Euler [5]  $y_{i+1} = y_i + h_t f(t_i, y_i)$   $y_{i+1} = y_i + h_t \left(Ay_i + F_i\right)$   
Midpoint rule [6]  $y_{i+2} = y_i + h_t + f\left(t_{i+1}, \frac{1}{2}(y_i + y_{i+2})\right)$   $y_{i+2} = (I - Ah_t) \setminus \left(y_i + 2h_t\left(\frac{Ay_i}{2} + F_{i+1}\right)\right)$ 

Table 3.1: Proposed methods for integrating in time. A problem that arises with the midpoint rule is the need to know  $F_{i+\frac{1}{2}}$ , this is solved by doubling the step size. Er denne tabellen fin nok?



(a) Help line decreases with  $m^2$ . (b) Help line decreases with m. (c) Help line decreases with  $m^2$ .

Figure 3.1: Figure of the convergence for the different integration methods. !!!!!!!Skrive inn det somstår på toppen av figuren her!!!!!

Figure 3.1 shows that all figures converge with the expected rate.

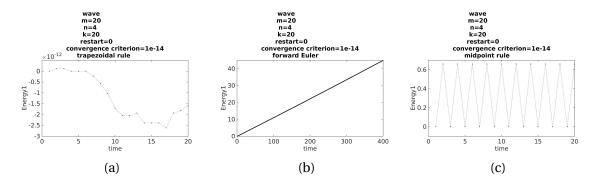


Figure 3.2: Figure of the difference in energy at a point in time. It is clear that only trapezoidal rule gives a suitable approximation of the error. Forward euler has an linearly increasing energy, while the midpoint rule gives periodic energy. Skrive inn det som står på toppen av figuren her

After looking at figure 3.2 it is easy to conclude that trapezoidal rule outperforms the other two integration methods.

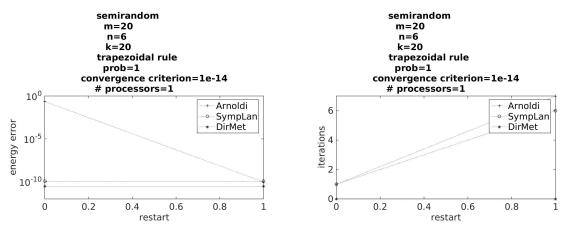
### **Energy preservation for SLM**

It can be proved that a restart of SLM does not alter the energy. This chapter is devoted to showing that this still hold with numerical approximations.

The residual energy of the symplectic Lanczos method is

$$\frac{1}{2}e_r^{\top} J A e_r + e_r^{\top} J r_{n+1} e_{2n}^{\top} z \tag{4.1}$$

with  $e_r = u - u_n$  (analytical solution minus approximated solution) and  $r_{n+1}$  is the residual vector given by the symplectic Lanczos method.



restart.

(a) The difference in energy with and without (b) The number of iterations performed with and without restarting.

Figure 4.1: The figure shows how the different methods change the energy with and without restarting.

The figures above implies that restarting the symplectic Lanczos method does indeed not change the energy. But for Arnoldi's method it changes quite a bit.

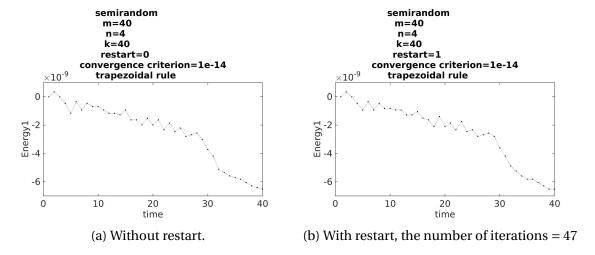


Figure 4.2: The figures shows the change in energy over time. Mer tekst

The figure above shows very little change in energy with SLM, with and without several restarts.

The figures below shows the same as figure 4.2, but with KPM instead of SLM.

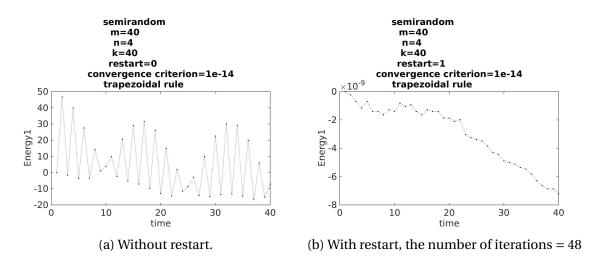


Figure 4.3: Figures showing the change in energy over time. Mer tekst

When comparing figure 4.2a and 4.2b it becomes clear that SLM's does not alter the energy significantly when performing the restart. Figure 4.3a and 4.3b shows that this is not the case

for	KD	M
1111	$\mathbf{r}$	IVI.

# Some interesting results

We will now show some numerical experiments using a randomly generated Hamiltonian matrix(semirandom).

### **Bibliography**

- [1] Sindre Ekslenad. A krylov projection method for the heat equation.
- [2] Heike Faßbender Peter Benner. An implicitly restarted symplecuc lanczos method for the hamlltonlan eigenvalue problem. *LINEAR ALGEBRA AND ITS APPLICATIONS 263:75-111*, 1997.
- [3] Martin Stoll Peter Benner, Heike Faßbender. A hamiltonian krylov–schur-type method based on the symplectic lanczos process. *Linear Algebra and its Applications*, (435):578–600, 2011.
- [4] Endre Süli and David F. Mayers. *An Introduction to Numerical Analysis*, chapter 7.2 Newton–Cotes formulae, pages 202–203. cambridge university press, 2003.
- [5] Endre Süli and David F. Mayers. *An Introduction to Numerical Analysis*, chapter 12.2 Onestep methods, page 317. cambridge university press, 2003.
- [6] Endre Süli and David F. Mayers. *An Introduction to Numerical Analysis*, chapter Definition 10.1, page 286. cambridge university press, 2003.
- [7] Saad Yousef. *Iterative Methods for Sparse Linear Systems*, volume SECOND EDITION, chapter 6.3.1, page 154. Siam, 2003. Algorithm 6.1.