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Projection methods for Hamiltonian systems

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Preface

This is a master thesis as a part of the study program industrial mathematics. It was written during the winter 2015-2016.

Acknowledgment

Thanks to Elena Celledoni for guiding me, and Lu Li for giving me the theoretical insight this text needed.

Summary and Conclusions

To be filled in!

Contents

Preface i

Acknowledgment ii

Summary and Conclusions iii

1 Introduction **2**

2 TTD **3**

3 Theory **4**

3.1 Discretization 4

3.2 Zero initial condition 6

3.3 Dividing the time domain 7

3.4 Energy 8

3.5 Integration methods 8

3.6 Abbriviations 8

3.7 Implementation 8

3.8 Solution methods 9

3.8.1 Arnoldi's Algorithm and the Krylov projection method 10

3.8.2 Symplectic Lanczos method 12

3.8.3 Direct method 14

3.8.4 Number of operations 15

4 Results **17**

4.1 Convergence 17

4.1.1 Hamiltonain system 17

4.1.2 Non-Hamiltonian system . . . 18
4.2 Integration method . . . 18
4.2.1 Hamiltonian system . . . 19
4.2.2 Non-Hamiltonian system . . . 20
4.3 Energy preservation for SLM . . . 20
4.3.1 Constant energy . . . 20
4.3.2 Varying energy . . . 22
4.4 Run time comparison . . . 22
4.4.1 constant energy . . . 23
4.4.2 Varying energy . . . 23
4.5 Something with slm and energy differnent times . . . 24
4.6 K versus k . . . 27
4.6.1 Constant energy . . . 27
4.6.2 Varying energy . . . 28
4.7 The perfect restart variable . . . 28
4.7.1 Constant energy . . . 29
4.7.2 Varying energy . . . 31
4.8 Integrating over looong time . . . 32
4.8.1 Constant energy . . . 33
4.8.2 Varying energy . . . 34

Chapter 1

Introduction

The equation

$$\begin{aligned} \dot{u}(t) &= Au(t) + p \cdot f(t) = g(t) \\ u(0) &= u_0 \end{aligned} \tag{1.1}$$

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) [2], which uses Arnoldi's algorithm(Arnoldi) as orthogonalisation method. This note will continue on the same track, but with more focus on Hamiltonian discretizations of wave equations, random problems, and energy preservation. It will also feature a comparison between symplectic Lanzcos method(SLM) [6] and Arnoldi. SLM is a projection technique that only works on Hamiltonian matrices. Due to this, SLM (claims to) preserve energy better than Arnoldi. This note will also compare time consumption and global error for the different methods, but will not contain much theoretical derivation. For this I recommend reading [1], [2], [6], [5], and [3].

There will also be a comparison between some different integration methods, and how the projection methods change when the time domain is divided into smaller pieces and each piece is considered independently with initial conditions from previous time domain.

Chapter 2

TTD

- Jeg synes at som minimum i oppgaven din burde du klare å avgjøre om SLM med restart er energibevarende eller ikke og om den gir lineæar vekst av globalfeil eller raskere vekst.
- Skrive bilde text, og fjerne lables fra bilder!
- Bevise at det er lurt å sammenligne KPM/SLM med DM?.
- SKrive mer generelt
- Er det flere figurer jeg burde ha med?
- Rekkefølgen må fikses
- Fix notasjon
- Skriv om error
- Skriv litt om antall matematiske operasjoner hver metode trenger
- Sett parantes rundt iterasjonsvariabler på z-er, og endre z-er til ϵ og δ?
- Forandre slim at SLM og SLPM er noe greier!!!!!!!!!!
- Forklare hva Hamiltonsk betyr og noe slikt!

Chapter 3

Theory

There will here be a short explanation of all solvers, constants, abbreviations and expressions used in this text. MATLAB notation is used where applicable.

3.1 Discretization

Divide each spacial direction in m pieces, with step size $h_s = 1/m$. The number of steps in time is denoted by k, making the step size in time, $h_t = 1/k$.

Let the matrix I_j be the identity matrix with dimension j, and let

$$J_j = \begin{bmatrix} 0 & I_j \\ -I_j & 0 \end{bmatrix}. \tag{3.1}$$

Equation (1.1) can be the result of several discretized equations. Since SLM needs a Hamiltonian matrix this will be the main focus. Two different matrices was implemented, with some test problems.

The first is the 2 dimensional wave equation,

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + f(t,x,y). \tag{3.2}$$

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

$$\begin{aligned} \tilde{A} &= \frac{2}{h_s^2}\,\text{gallery}('\text{poisson}', m-2) \\ A &= \begin{bmatrix} 0 & I_{\hat{m}} \\ -\tilde{A} & 0 \end{bmatrix} \end{aligned} \quad . \tag{3.3}$$

The matrix $\tilde{A}$ is also known as the five-point stencil[4]. This matrix will be referred to as `wave`. The second implemented Hamiltonian matrix is random, and given by

$$\begin{aligned} \hat{A} &= \text{rand}(\hat{m}) \\ A &= \frac{1}{2} J_{\hat{m}} \cdot (\hat{A} + \hat{A}^\top + m^2 I_{\hat{m}}). \end{aligned} \tag{3.4}$$

Since we are interested in comparing the different projection methods to each other, the matrix will be saved and reused. This matrix will be referred to as `semirandom`. The part $m^2 I_{\hat{m}}$ is added to make $J_{\hat{m}} A$ diagonally dominant, since a fully random problem will not converge in general. The matrix is simulated as a 2 dimensional system.

These two matrices also has some test problems that satisfies the conditions

$$u(t,0,y) = u(t,1,y) = u(t,x,0) = u(t,x,1) = 0.$$

The test problems will be divided in two cases. One where the energy is constant, and one where the energy is varying.

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

$$\begin{aligned} u(t,x,y) &= \sin(\pi x)\sin(\pi y)\cos(\sqrt{2}\pi t) \\ u_0(x,y) &= \sin(\pi x)\sin(\pi y) \\ f(t,x,y) &= 0, \end{aligned} \tag{3.5}$$

and

$$\begin{aligned} u(t,x,y) &= \text{unknown} \\ u_0(x,y) &= \text{rand}(2(m-2)^2,1) \\ f(t,x,y) &= 0 \end{aligned} \tag{3.6}$$

for `semirandom`.

In the case with varying energy and `wave` is used the test problem is !!!!!!!!!!!!!!!!!!!!!!!!!!Jeg bruker et annet testproblem nå!!!!!!!!!!!!!!!!!!!!!!!!!!!

$$\begin{aligned} u(t,x,y) &= (x-1)x(y-1)y(t^2-t+1) \\ u_0(x,y) &= (x-1)x(y-1)y \\ f(t,x,y) &= 2(y(y-1)+x(x-1))\cdot\big(-(t^2-t+1)\big), \end{aligned} \tag{3.7}$$

and

$$\begin{aligned} u(t,x,y) &= \text{unknown} \\ u_0(x,y) &= 0 \\ f(t,x,y) &= \text{rand(1,k)}\cdot\text{rand}(2(m-2)^2,1), \end{aligned} \tag{3.8}$$

for `semirandom`. When using one of the projection methods f needs to be separable in time and space. In the case where f is not separable it is not recommended to use this method, see [2] for more information.

The test problems are discretized with $y_i = ih_s$, $x_i = ih_s$ and $t_j = jh_t$ with $i = 1,2,\cdots,m-1$ and $j = 1,2,\cdots,k$. The time discretized solution of u will be called U.

3.2 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: Start by shifting the solution

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

then rewrite the original equation as

$$\dot{\hat{u}}(t) = A\hat{u}(t) + Au_0 + F(t)$$
$$\hat{u}(0) = 0.$$

The equation above solves the shifted problem, solve the original problem by shifting it back with

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

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

!!!!!!!!!!!!!!!!!!!!!!!!Skriv at det er vanskelig å sammenligne med `semirandom` fordi man ikke vet den ordentlige løsningen!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

3.3 Dividing the time domain

!!!!!!!!!Forklar hvorfor dette er noe vil vil gjøre(jeg forstår det ikke nå)!!!!!!!!!

Let T_s denote simulated time, let K be the number of pieces T_s is divide into, and let k be the number of pieces each K is divided into. The procedure is to solve each of the K intervals as separate problems, with the initial conditions updated. This is explained in a more precise manner in algorithm 1.

Algorithm 1 !!!!!!!Spør elena om dette har et fint navn jeg kan bruke!!!!

Start with an initial value U_0, K and k.
Make an empty vector u
for $j = 1, 2, \cdots, K$ **do**
  Solve differential equation with $k+1$ points in time and initial value U_0
  Place the new points at the end of u.
  Update U_0 to be the last value of u
  Delete the last point of u
end for
Return u.

Trapezoidal rule [7]	$U_{i+1} = U_i + h_t g\left(\frac{1}{2}(t_i + t_{i+1}), \frac{1}{2}(U_i + U_{i+1})\right)$ $U_{i+1} = (I - \frac{Ah_t}{2})^{-1}\left(U_i + \frac{h_t}{2}\left(AU_i + (F_{i+1} + F_i)\right)\right)$
Forward Euler [8]	$U_{i+1} = U_i + h_t g(t_i, U_i)$ $U_{i+1} = U_i + h_t\left(AU_i + F_i\right)$
Midpoint rule [9]	$U_{i+1} = U_i + h_t g\left(t_{i+\frac{1}{2}}, \frac{1}{2}(U_i + U_{i+1})\right)$ $U_{i+\frac{1}{2}} = U_i + \frac{h_t}{2}(AU_i + F_{\frac{1}{2}})$ $U_{i+1} = (I - \frac{Ah_t}{2})^{-1}(U_{i+\frac{1}{2}} + \frac{h_t}{2}F_{i+\frac{1}{2}})$

Table 3.1: Methods for integrating in time. Note that since the midpoint rule uses $F_{i+\frac{1}{2}}$ we need to save twice as many points for midpoint rule, as for the other methods.

3.4 Energy

!!!!!!!!!!!!!!!!!!!!!!SKRIV bedre her!!!!!!!!!!!!!!!!!!!!!!!!

The energy for a system on the form of equation 1.1 is [3]

$$\mathcal{H}(t) = \frac{1}{2}u(t)^\top JAu(t) \tag{3.9}$$

This energy is the

3.5 Integration methods

The integration considered in this text are trapezoidal rule, forward euler, and midpoint rule. The definition and the iteration scheme of the different methods are given in table 3.1.

3.6 Abbriviations

Table 3.2 contains an explanation of the expressions you will see on figures later.

3.7 Implementation

!!!!!!!!!!!!!!!!!!!!!!SKRIV bedre her!!!!!!!!!!!!!!!!!!!!!!!!

All algorithms and methods was made in matlab R2014b on an ubuntu 14.04 LTS computer with

r_n	Number of restarts performed by Arnoldi or symplectic Lanczos method.
T_c	Computation time used to solve a problem
er_1	Difference between analytical solution, and orthogonalised solution.
en_1	Difference in energy between analytical solution, and orthogonalised solution.
er_2	Difference between orthogonalised solution, and the non-orthogonalised solution.
en_2	Difference in energy between orthogonalised solution, and the non-orthogonalised solution.
m	Number of point in each spacial direction
n	Size of orthogonal space, also called restart variable
k	Number of points in time
T_s	Simulated time
`restart`	A boolean value. If `restart` == 1, Arnoldi or symplectic Lanczos method will restart.
ϵ	If `restart` is true, restarting will commence until the change in the solution is less than ϵ

Table 3.2: Explanation of abbreviations.

intel i7 4770 CPU and 16 GB of RAM. Matlab's backslash operator was used to solve the linear system in trapezoidal rule, and midpoint rule.

!!!!!!!!!!!Skrive hvordan bilder er laget!!!!!!!!!!!

!!!!!!!!!!!!!Skrive hvordan funksjoner er implementert!!!!!!!!!!!!!!!!!

!!!!!!!!!!!!!Skrive hvordan ting er sammensatt!!!!!!!!!!!!!!!!!

3.8 Solution methods

!!!!!!!!!!!!!!!!!!!Forklar iterasjonsvariablen i!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

There are two orthogonalisation methods that will be discussed in this text. Their names are symplectic Lanczos method, and Arnoldi's algorithm. This section will only contain some of the key points that makes these algorithms work.

!!!!!!!!!Skriv hva projeksjonemetoder er!!!!!!!!!!!!!

Projection methods are ways to make an approximated solution from a subset of the original problem. One great feature of these methods is that a smaller system of equations can be used to obtain solutions, the drawback is that the solutions are approximated and that the orthogonal

system needs to be found, and this can be time consuming. The approximated solution can be improved by restarting, this means using the projection method again, and solve an equation for the difference between the projected solution, and the true solution repeatedly.
!!!!!!!!!!!!!!!! forkalr restart bedre?!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

Assume that equations on the form

$$\begin{aligned} \dot{u}(t) &= Au(t) + p \cdot \tilde{f}(t) \\ u(0) &= u_0 \end{aligned} \tag{3.10}$$

is written as

$$\begin{aligned} \dot{u}(t) &= Au(t) + v \cdot f(t) \\ u(0) &= 0 \end{aligned} \tag{3.11}$$

when these methods are used, note that the initial values are zero. It is also important that A is a Hamiltonian matrix when using SLM.

Note that the relation between $\hat{m}$, $\tilde{n}$, $\tilde{m}$ used in the algorithms is given by $\hat{m} = 2\tilde{m} = 2(m-2)^2$ and $n = 2\tilde{n}$. Don't worry to much about these details, it is just a way to simplify the expressions.

3.8.1 Arnoldi's Algorithm and the Krylov projection method

This section is loosely based around the derivation of the method done in [**?**].

The Krylov subspace is the space $W_n(A, v) = \{v, Av, \cdots, A^{n-1}v\} = \{v_1, v_2, \cdots, v_n\}$, where $n \leq \hat{m}$. The vectors v_i together with $h_{i,j} = v_i^\top A v_j$, are found by using Arnoldi's algorithm, shown in algorithm 2. Let V_n be the $\hat{m} \times n$ matrix consisting of column vectors $[v_1, v_2, \cdots, v_n]$ and H_n be the $n \times n$ upper Hessenberg matrix containing all elements $(h_{i,j})_{i,j=1,\cdots,n}$. Then the following holds [**?**]

$$\begin{aligned} AV_n &= V_n H_n + h_{n+1,n} v_{n+1} e_n^\top \\ V_n^\top A V_n &= H_n \\ V_n^\top V_n &= I_n. \end{aligned} \tag{3.12}$$

Algorithm 2 Arnoldi's algorithm[10]

Start with $A \in \mathbb{R}^{\hat{m}\times\hat{m}}$, $v \in \mathbb{R}^{\hat{m}}$, $n \in \mathbb{N}$ and $\epsilon \in \mathbb{R}$.
$v_1 = v/\|v\|_2$
for $j = 1,2,\cdots,n$ **do**
  Compute $h_{i,j} = v_i^\top A v_j, v_i$ for $i = 1,2,\cdots,j$
  Compute $w_j = Av_j - \Sigma_{i=1}^{j} h_{i,j} v_i$
  $h_{j+1,j} = \|w_j\|_2$
  if $h_{j+1,j} < \epsilon$ **then**
    STOP
  end if
  $v_{j+1} = w_j / h_{j+1,j}$
end for
Return H, V, v_{n+1}, $h_{n+1,n}$.

Here, e_n is the nth canonical vector in $\mathbb{R}^n$. n is the number of iterations Arnoldi ran, also called the restart variable.

By using the transformation $u(t) \approx V_n z_n^i(t)$, equation (3.11) can, with the help of equation (3.12) be written as

$$\begin{aligned} \dot{z}_n^0(t) &= H_n z_n^0(t) = \|v\|_2 e_1 f(t) \\ z_n^0(0) &= 0. \end{aligned} \tag{3.13}$$

The approximated solution of the original problem can be attained by the following relation

$$u(t) \approx V_n z_n^i(t). \tag{3.14}$$

The derivation of the method is shown in [**?**]. Here it is shown that larger n gives a better approximation of the solution, but larger n also gives higher computational complexity, see [**?**] for proof of convergence. The drawback is also that there is no way of knowing in advance how well the approximation will be, but the size of $h_{n+1,n}$ does say something about how well the solution

is approximated, smaller $h_{n+1,n}$ means a smaller error. If the approximation is not sufficient the solution must be recalculated with larger n, unless you perform a restart.

The restart considers the difference between $V_n z_n^0(t)$ and $u(t)$, as in equation (3.15).

$$\left(V_{\hat{m}} z_{\hat{m}} - V_n^i z_n^i\right)'(t) = A\left(V_{\hat{m}} z_{\hat{m}} - V_n^i z_n^i\right)(t) - r_n^i \tag{3.15}$$

where

$$r_n^i(t) = v^{i-1} f(t) - V_n^{i-1} \dot{z_n}^{i-1}(t) + A V_n^{i-1} z_n^{i-1}(t) = h_{n+1,n}^{i-1} e_n^\top z_n(t)^{i-1} v_{n+1}^{i-1} \tag{3.16}$$

This expression can be simplified by using equation (3.12) to look like equation (3.17).

$$\dot{z}_n^i(t) = H_n z_n^i(t) + h_{n+1,n}^{i-1} e_n^\top z_n^{i-1}(t), \quad i \geq 1 \tag{3.17}$$

This equation can be repeatedly solved, and increase the accuracy of the approximated solution within an arbitrary constant of the true solution. This equation works for $i = 1, 2, \cdots$, the 0th iteration is done by equation (3.13). It is no longer possible to use $h_{n+1,n}$ as a measure for the error when the restart is used, so other ways of finding the error must be used.

If you want to derive this yourself, note that the z_n^1 in equation (3.17) is defined as the difference between $z_n^0(t)$ and $z_{\hat{m}}^0(t)$. The derivation of the method can be found in [**?**].

The proof for the convergence of the restart can be found in [**?**].
!!!!!!!!!!!!!!!!!!Flytt algoritmene!!!!!!!!!!!!!!!!!!!!!!!

3.8.2 Symplectic Lanczos method

!!!!!!!!!!!Sjekk dimensjoner på alt jeg skriver om her!!!!!!!!!!!!!!!!!!!
SLM and KPM are very similar, which is easy to see when comparing equation (3.12) and (3.18). The main difference is that orthonormality in Arnoldi is replaced by symplecticity in SLM. This makes the derivation quite similar.

Let $S_n = [v_1, v_2, \cdots v_{\frac{n}{2}}, w_1, w_2, \cdots w_{\frac{n}{2}}]$ be a set of J-orthogonal vectors satisfying the following equations

$$\begin{aligned} AS_n &= S_n H_n + h_{n+1,n} v_{n+1} e_{\hat{m}}^\top \\ J_{\hat{m}}^{-1} S_n^\top J_n A S_n &= H_n \\ S_n^\top J_n S_n &= J_{\hat{m}} \end{aligned} \tag{3.18}$$

!!!Endre nevnene på variablene!!!!!!!!!!!!!

Algorithm 3 Symplectic Lanczos method [6], with reortogonalization from [5].

Start with a Hamiltonian matrix $A \in \mathbb{R}^{2\tilde{m}\times 2\tilde{m}}$, $\tilde{v_1} \in \mathbb{R}^{2\tilde{m}}$, $\tilde{n} \in \mathbb{N}$
$v_0 = 0 \in \mathbb{R}^{2\tilde{m}}$
$\zeta_1 = \|\tilde{v}_1\|_2$
$v_1 = \frac{1}{\zeta_1}\tilde{v}_1$
for $j = 1, 2, \cdots, \tilde{n}$ **do**
  $v = Av_j$
  $\delta_j = v_j^\top v$
  $\tilde{w} = v - \delta_j v_j$
  $\kappa_j = v_j^\top J_{\tilde{m}} v$
  $w_j = \frac{1}{\kappa_j}\tilde{w}_j$
  $w = Aw^j$
  $\tilde{V}_{j-1} = [v_1, v_2, \cdots, v_{j-1}, w_1, w_2, \cdots, w_{j-1}]$
  $w_j = w_j + \tilde{V}_{j-1} J_{j-1} \tilde{V}_{j-1}^\top J_{\tilde{m}} w_j$
  $\beta = -w_j^\top J_{\tilde{m}} w$
  $\tilde{v}_{j+1} = w - \zeta_j v_{j-1} - \beta_j v_j + \delta_j v_j$
  $\zeta_{j+1} = \|\tilde{v}_{j+1}\|_2$
  $v_{j+1} = \frac{1}{\zeta_{j+1}}\tilde{v}_{j+1}$
  $\tilde{V}_j = [v_1, v_2, \cdots, v_j, w_1, w_2, \cdots, w_j]$
  $v_{j+1} = v_{j+1} + \tilde{V}_j J_j \tilde{V}_j^\top J_{\tilde{m}} v_{j+1}$
end for
$V = [v_1, v_2, \cdots, v_{\tilde{n}}, w_1, w_2, \cdots, w_{\tilde{n}}]$
$H = \begin{bmatrix} \text{diag}\big([\delta_j]_{j=1}^n\big) & \text{tridiag}\big([\zeta_j]_{j=2}^n, [\beta_j]_{j=1}^n, [\zeta_j]_{j=2}^n\big) \\ \text{diag}\big([\kappa_j]_{j=1}^n\big) & \text{diag}\big([-\delta_j]_{j=1}^n\big) \end{bmatrix}$
Return H, V, v_{n+1}, ζ_{n+1}.

Here S_n is an $\hat{m} \times n$ matrix, H_n is an $n \times n$ matrix, where $\frac{n}{2}$ is the number of iterations the algorithm performed, this is because the algorithm makes two vectors per iterations, v and w.

The process of making the vectors and matrix is a little more involved than for Arnoldi's algorithm, so there will be no thorough explanation of how it works, except for in Algorithm 3.

The reduced system, given in equation 3.19, is found by substituting $u(t) \approx S_n z(t)$, as in Arnoldi, and use equation (3.18).

$$\dot{z}^0 = H_n z_n^0 + (J_n)^{-1} S_n J_{\hat{m}} A v \tag{3.19}$$

A restart can also here be performed if the accuracy of the solution is not satisfactory. This can be derived by looking at the difference between $V_n z_n(t)$ and $u(t)$, the result is given in equation (3.20).

$$\begin{aligned} \dot{z}_n^i = H_n^i z_n^i + J_n^{-1} {S_n^i}^\top J_{\hat{m}} \zeta_{n+1}^{i-1} v_{n+1}^{i-1} e_n^\top z_n^{i-1}, \quad i \geq 1 \\ z_n(0) = 0 \end{aligned} \tag{3.20}$$

For the derivation of the method see [**?**]. As for Arnoldis algorithm, $z_n^i, i \geq 1$ is renamed to be the difference between $V_n z_n(t)$ and $u(t)$.

Proof of convergence and other interesting results for this method can be found in [**?**].

3.8.3 Direct method

It is important to have some method to compare with. This will be done by solving the problem without using any of the projection methods. It is easy to show that when solving a problem with any of the projection methods presented here you are trying to approximate the solution obtained without using a projection method. This is also the best any projection method can do. Thus direct method, or `DM` as it will be called in this text, is the natural comparator for these projection methods.

Operation	Cost
Integration with forward Euler	$\mathcal{O}(kn^2)$
Integration with Trapezoidal or midpoint rule	$\mathcal{O}(kn^3)$
Arnoldi's algorithm	$\mathcal{O}(n^2m)$
Symplectic Lanczos method	$\mathcal{O}(nm^2)$
Transforming from $z_n(t)$ to $u(t)$	$\mathcal{O}(mnk)$
Matrix vector multiplication (sparse matrix)	$\mathcal{O}(m)$
Matrix vector multiplication (dense matrix)	$\mathcal{O}(m^2)$

Table 3.3: Computational cost of some mathematical operations. !!!!!!!!!!!!!!!!!!Husk å cite alt!!!!!!!!!!!!!!!

Method	Number of operation
KPM	$\mathcal{O}((n^2m + kn^3 + mnk)\gamma)$
SLM	$\mathcal{O}((nm^2 + kn^3 + mnk)\gamma)$
DM	$\mathcal{O}(km^3)$

Table 3.4: Number of operations needed for the different methods. γ is the number of restarts needed for the method to converge.
!!!!!!!!!!!!!!!!!Sjekk disse resultatene!!!!!!!!!!!!!!
!!!!!!!!!!!!Husk å cite alt!!!!!!!!!!!!!!!

3.8.4 Number of operations

Since computation times might be uncertain due to different additional loads (web surfing, writing and so on) there will here be a short comparison between the number of operations for each method. This will also give a basis for what to expect from the different methods.

A table of computational cost for different operations is given in table **??**. Sections **??** to 3.8.4 will contain a motivation for the results found in table **??**. It is assumed that trapezoidal method is used.

!!!!!!!!!!!!!!!!!!!Skriv mye her!!!!!!!!!!!!!!!!!!!!

KPM

KPM uses Arnoldi's algorithm, an integration method, and requires an additional mnk operations when transforming $V_n z_n(t)$ to $u(t)$.

SLPM

SLPM uses SLM, an integration method, transformation, and requires an additional m^2 operations to calculate $J^{-1}S_nJ\zeta\nu$, which is a matrix vector product, and S_n is a dense matrix. !!!!!!!!!!!!Forklar hvor de tallene kommer fra!!!!!!!!!!!!!!!!

DM

DM uses just an integration method, the downside is that $n = \hat{m}$.

Chapter 4

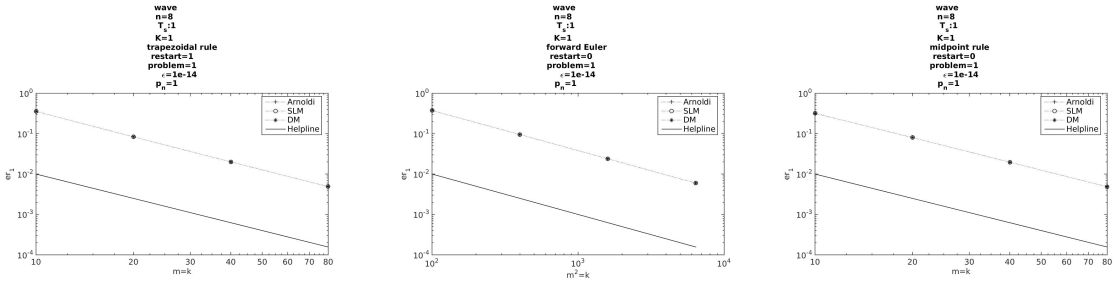
Results

!!!!!!!!Hint: kommenter ut bilder, få litt oversikt, og så legg til etterhvert som du går igjennom!!!!!!

4.1 Convergence

This section will show convergence of all the methods, with both Hamiltonian and non-Hamiltonian systems.

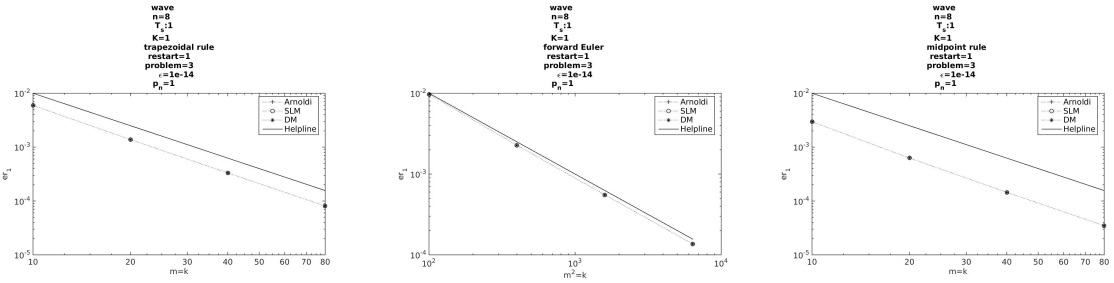
4.1.1 Hamiltonain system



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

Figure 4.1: Figure of the convergence for the different integration methods. All methods converge with the expected rate.

4.1.2 Non-Hamiltonian system



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

Figure 4.2: Figure of the convergence for the different integration methods. All methods converge with the expected rate.

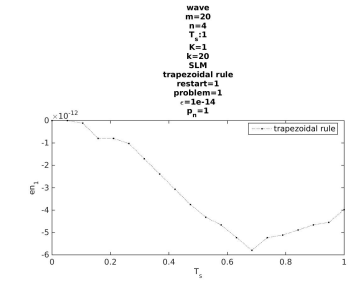
4.2 Integration method

This section will be concerned with comparing some different methods for integration in time.

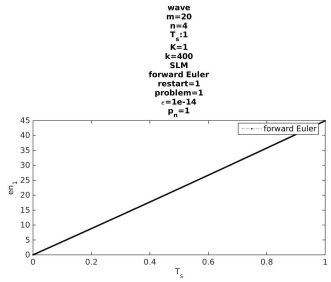
How well they estimate the error and energy will be the primary concern.

!!!!!!!!!!!!!!!!!!!!Her trengs det nye bilder!!!!!!!!!!!!!!!!!!!!!!

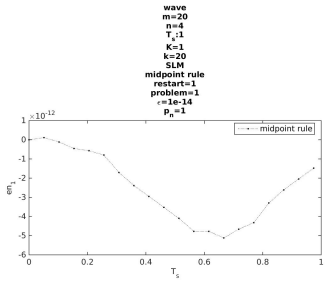
4.2.1 Hamiltonian system



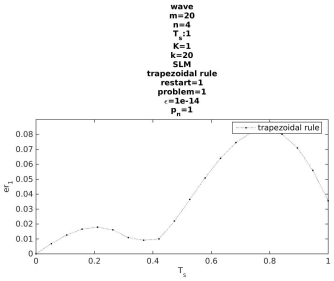
(a) Energy with trapezoidal rule.



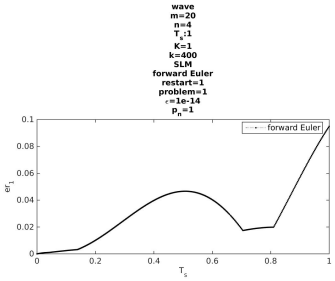
(b) Energy with forward Euler



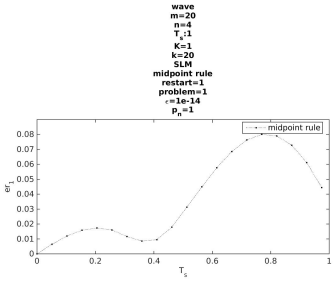
(c) Energy with midpoint rule



(d) Error with trapezoidal rule



(e) Error with forward Euler

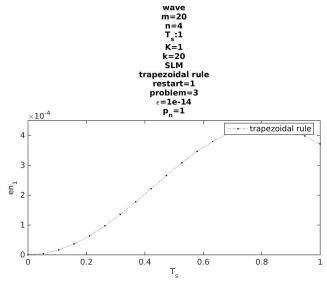


(f) Error with midpoint rule

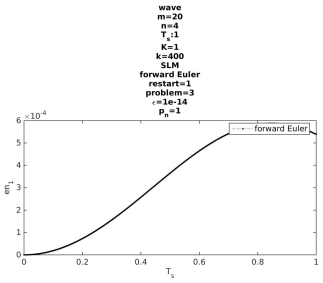
Figure 4.3: A snapshot of how energy and error changes over the simulated time with the different integration method without restart.

Both trapezoidal rule and midpoint rule to gives a very precise estimation of energy and error. Forward Euler on the other hand gives a linearly increasing energy, and with that a larger error, making it useless as an integration method in this case. The reason for the wired shapes in figure 4.3d and 4.3f is the periodicity of the test problem.

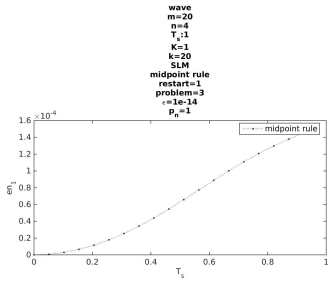
4.2.2 Non-Hamiltonian system



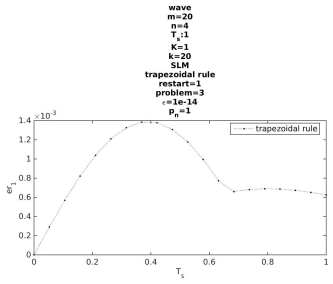
(a) Energy with trapezoidal rule.



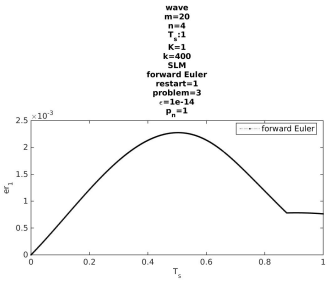
(b) Energy with forward Euler.



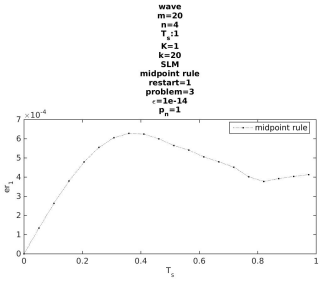
(c) Energy with midpoint rule.



(d) Error with trapezoidal rule.



(e) Error with forward Euler.



(f) Error with midpoint rule rule.

Figure 4.4: A snapshot of how energy and error changes over the simulated time with the different integration method without restart.
☿

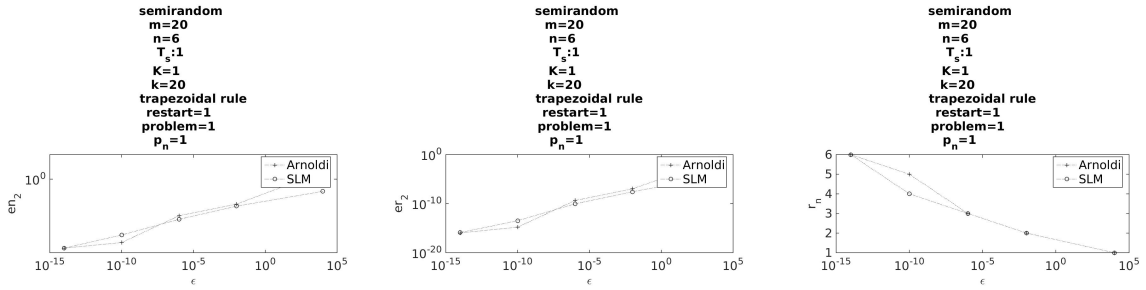
In this case all methods gives a suitable convergence for the error and the energy. There is no longer any problems with forward Euler's increasing energy. Again the shapes on the figures is a property of the test problems, and not a flaw in the method.

4.3 A closer look at SLM

Since SLM gives a symplectic matrix, the energy should not change with time. This section will be devoted to seeing how well this works in practice. There will also be a comparison about how the restart changes the energy preservation. In addition !!!!!!!!!!Bla bla bla!!!!!!!!!!!!!!!!!!!!

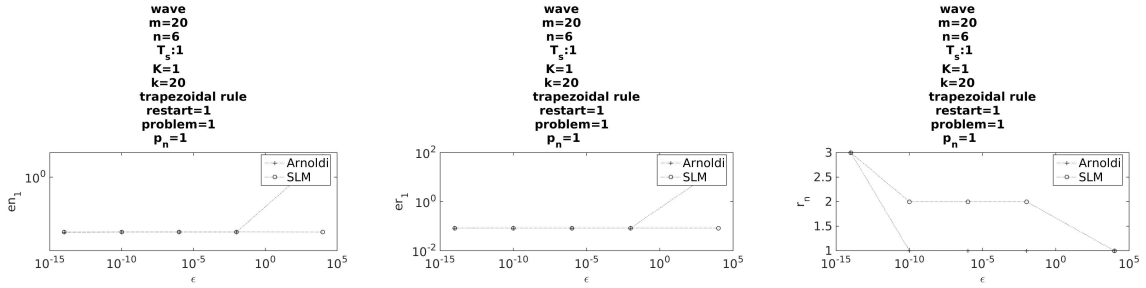
4.3.1 Constant energy

!!!!!!!!!!!!!!!!!!!!Det må skrives en del mer i dette kapitelet!!!!!!!!!!!!!!!!!!!!!!



(a) Energy. (b) Error. (c) Number of restarts.

Figure 4.5: The figure shows how the different methods change the energy and error with different number of restart for `semirandom`.



(a) Energy. (b) Error. (c) Number of restarts.

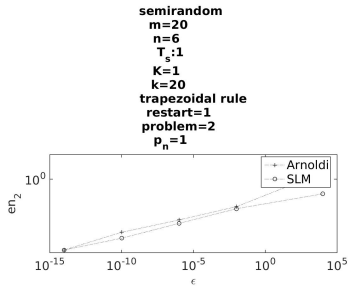
Figure 4.6: The figure shows how the different methods change the energy and error with different number of restart for `wave`.

There is a clear difference between how well the energy is estimated for `wave` and `semirandom`. For `semirandom` there is not much difference between SLM and Arnoldi, although SLM seams to give a slight better approximation than Arnoldi. With `semirandom` at $\epsilon = 10^{-10}$ Arnoldi preforms one more iteration than SLM, which makes it give a better approximation, aside from that SLM consistently preform better than Arnoldi.

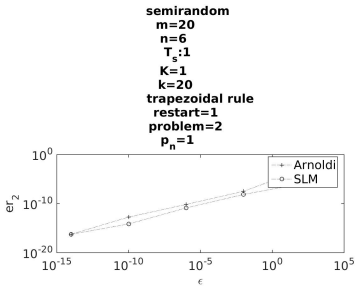
When comparing figure 4.5 and figure 4.6 it is important to remember that the way the er_1 and er_2 is found is very differently, and that might explain the why the cases differs so much. But the difference might also be explained with `semiradom` being a much harder equation to solve.

!!!!!!!!!!!!!!Skriv litt mer om hvorfor bildene for semirandom og wave er så forksjelkige!!!!!!!!!!!!!!!!!!!!!!

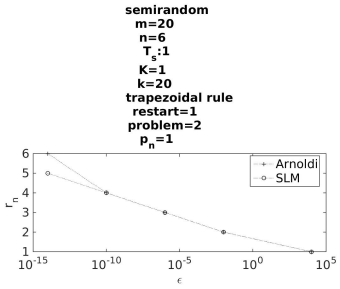
4.3.2 Varying energy



(a) The difference in energy with and without restart.

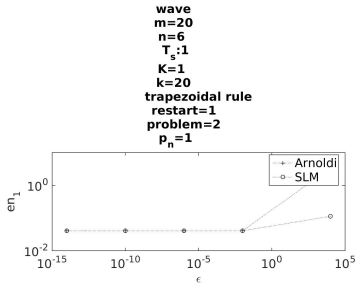


(b) The difference in energy with and without restart.

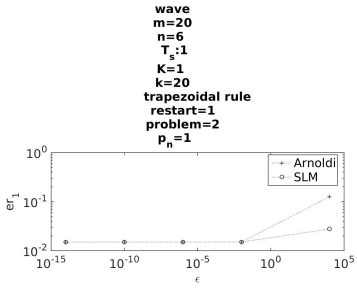


(c) The number of iterations performed with and without restarting.

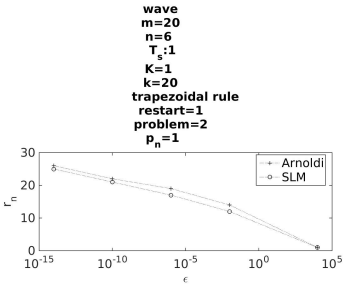
Figure 4.7: The figure shows how the different methods change the energy and error with different number of restart for `wave`.



(a) The difference in energy with and without restart.



(b) The difference in energy with and without restart.



(c) The number of iterations performed with and without restarting.

Figure 4.8: The figure shows how the different methods change the energy and error with different number of restart for `wave`.

The results here are very similar to the results found in section 4.3.1, except that the energy and error changes for the first points for both SLM and Arnoldi. SLM still gives the better approximation.

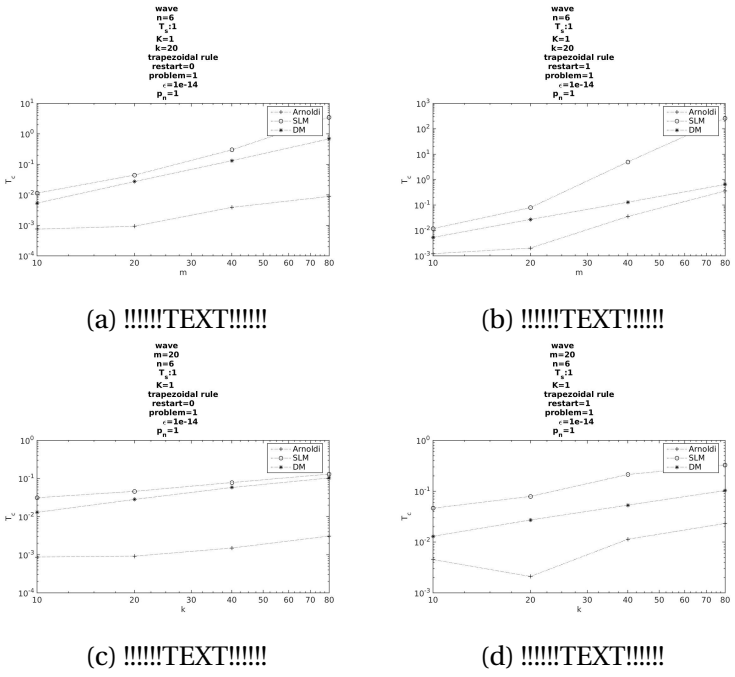
4.4 Run time comparison

!!!!!!!!!!!!!!!!!!!!!!!!!!Burde jeg ha med restart eller ikke på disse bildene?!!!!!!!!!!!!!!!!!

!!!!!!TEXT!!!!!!

4.4.1 constant energy

!!!!!!TEXT!!!!!!



(a) !!!!!!TEXT!!!!!! (b) !!!!!!TEXT!!!!!!

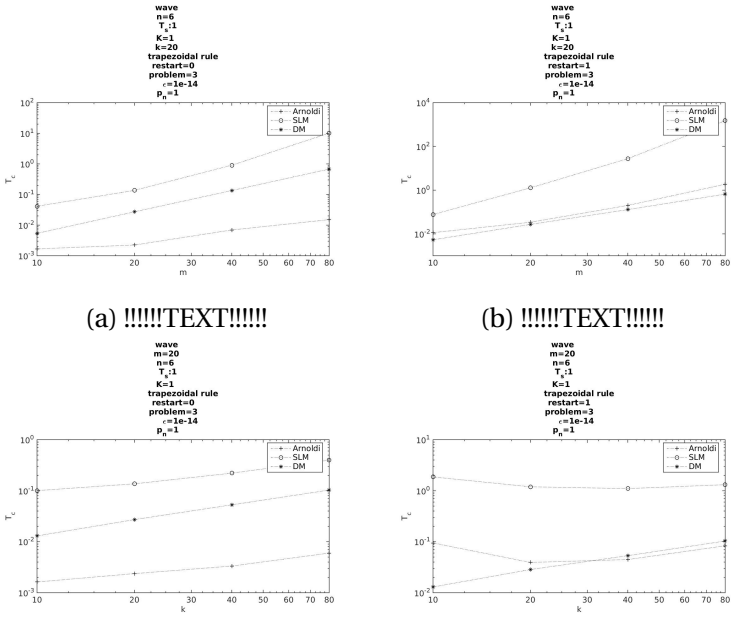
(c) !!!!!!TEXT!!!!!! (d) !!!!!!TEXT!!!!!!

Figure 4.9: !!!!!!TEXT!!!!!!

!!!!!!TEXT!!!!!!

4.4.2 Varying energy

!!!!!!TEXT!!!!!!



(a) !!!!!!TEXT!!!!!! (b) !!!!!!TEXT!!!!!!

(c) !!!!!!TEXT!!!!!! (d) !!!!!!TEXT!!!!!!

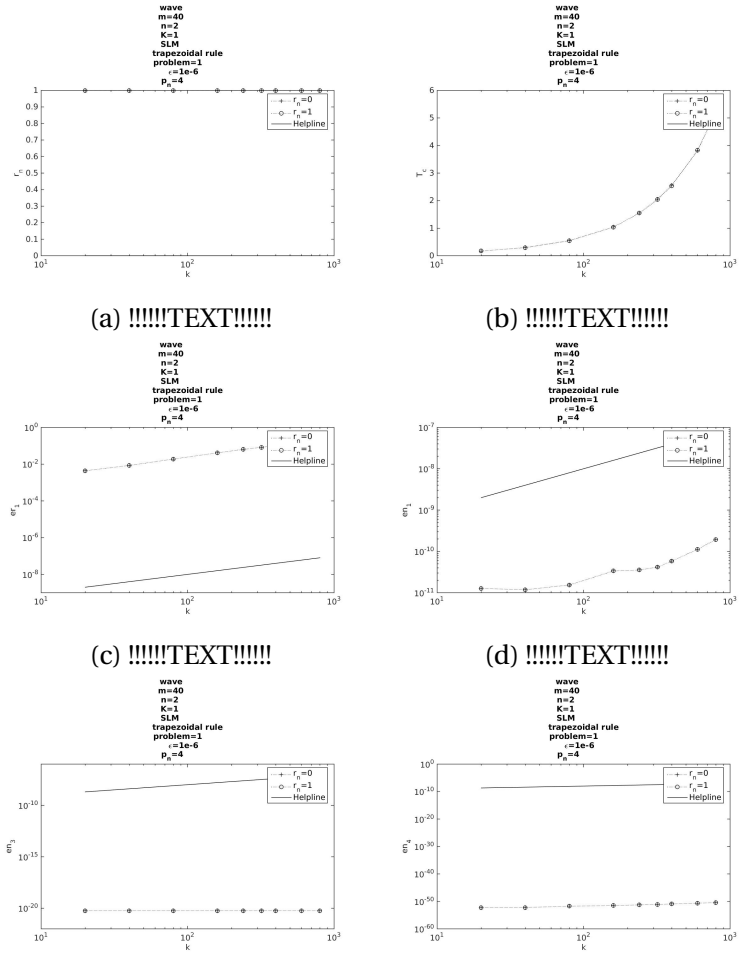
Figure 4.10: !!!!!!TEXT!!!!!!

!!!!!!TEXT!!!!!!

4.5 Something with slm and energy differnent times

!!!!!!!!!!!!!!!!Sett dette inn der det hører hjemme!!

!!!!!!!Text!!!!!!!!!!



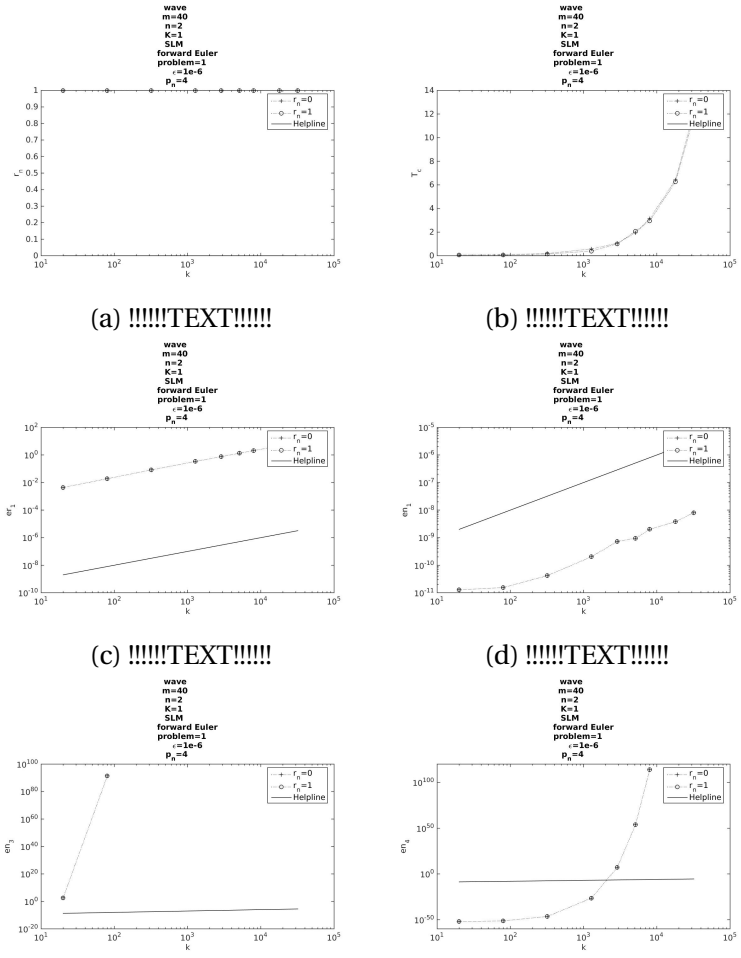
(a) !!!!!!TEXT!!!!!! (b) !!!!!!TEXT!!!!!!

(c) !!!!!!TEXT!!!!!! (d) !!!!!!TEXT!!!!!!

(e) !!!!!!TEXT!!!!!! (f) !!!!!!TEXT!!!!!!

Figure 4.11: !!!!!!TEXT!!!!!!

!!!!!TEXT!!!!!!!!!!!!!!!



(a) !!!!!!TEXT!!!!!! (b) !!!!!!TEXT!!!!!!

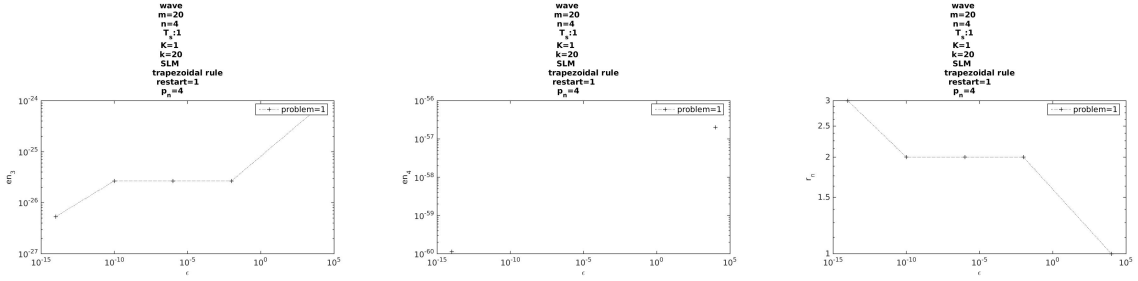
(c) !!!!!!TEXT!!!!!! (d) !!!!!!TEXT!!!!!!

(e) !!!!!!TEXT!!!!!! (f) !!!!!!TEXT!!!!!!

Figure 4.12: !!!!!!TEXT!!!!!!

!!!!!!!Text!!!!!!!!!!

$\mathscr{H}$



(a) !!!!!!TEXT!!!!!! (b) !!!!!!TEXT!!!!!! (c) !!!!!!TEXT!!!!!!

Figure 4.13: !!!!!!TEXT!!!!!!

4.6 K versus k

This method will now be tested, the goal is to see if the computation time can decrease without loosing precision in error or energy.

4.6.1 Constant energy

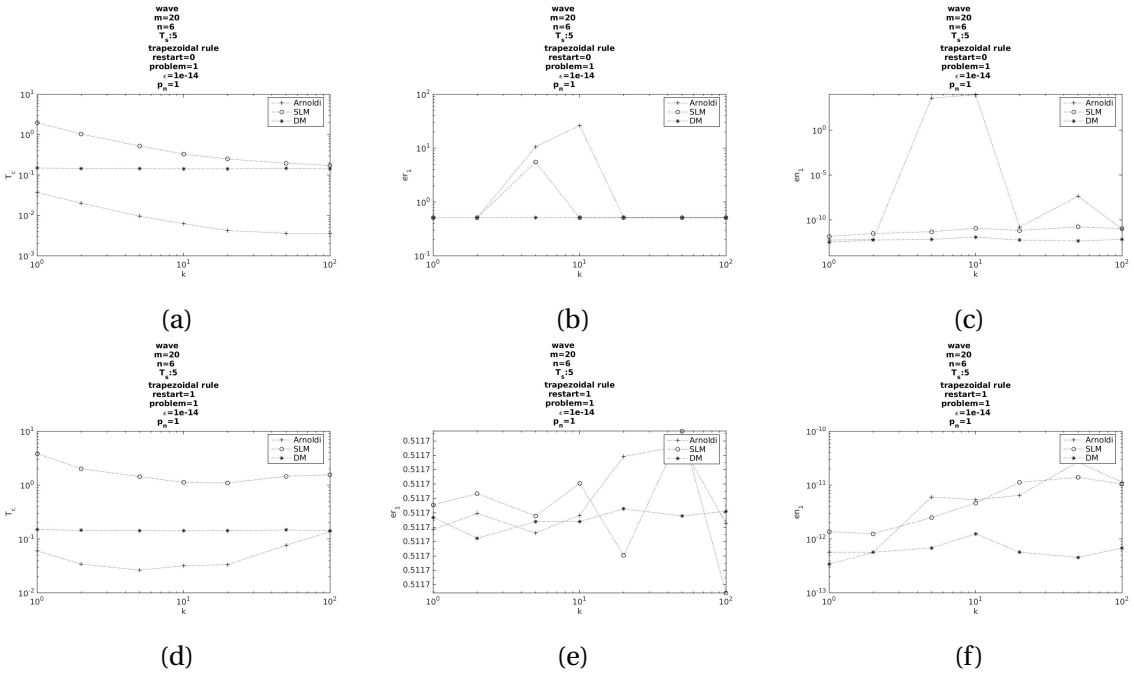


Figure 4.14: Figure showing how the different methods perform with different distribution of K and k. Notice that the product Kk is constant.

DM solving the equation with large K (and therefore smaller k) is faster, and gives no noticeable lack of precision in either energy and error. For Arnoldi and SLM there is not much to be gained computation time wise, notice also that when K is too large precision in energy and error is lost.

4.6.2 Varying energy

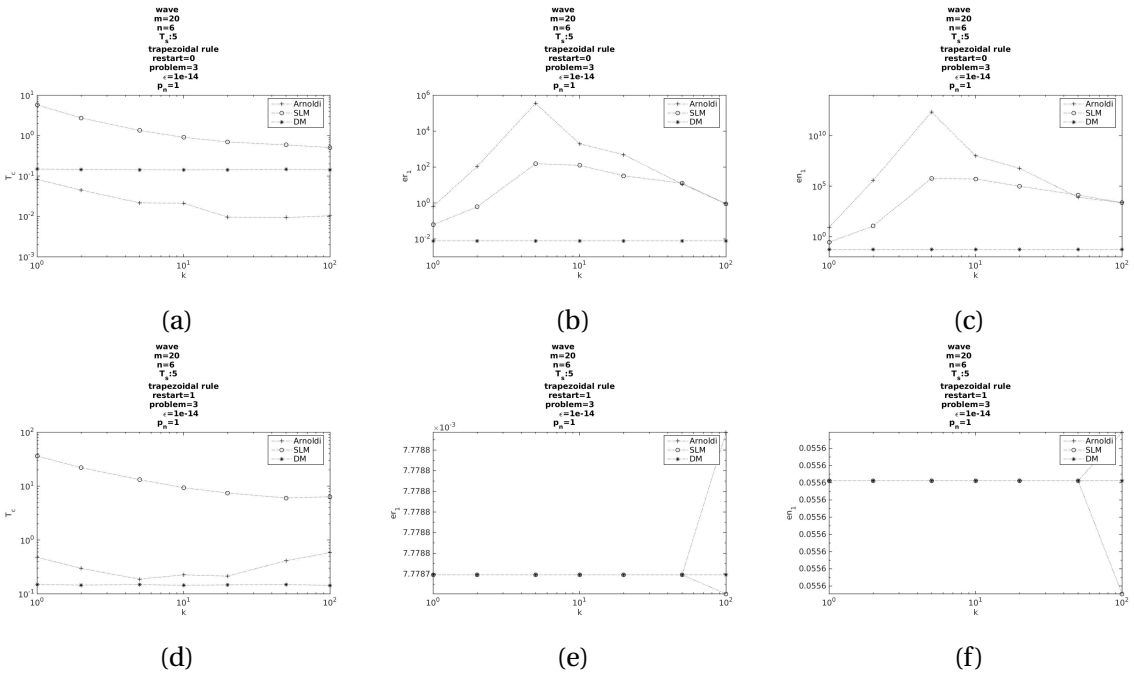


Figure 4.15: Figure showing how the different methods perform with different distribution of K and k. Notice that the product Kk is constant.

Figure 4.15 is very similar to figure 1. But there is here a definite decrease in computation time for SLM. Notice also that for larger K the energy and error diverges for both SLM and Arnoldi.

4.7 The perfect restart variable

The restart variable, denoted by n, is the size of the orthogonal system used with one of the projection method. Performing n iterations of Arnoldi's algorithm or $\frac{n}{2}$ iterations of SLM gives an orthogonal space of size n.

4.7.1 Constant energy

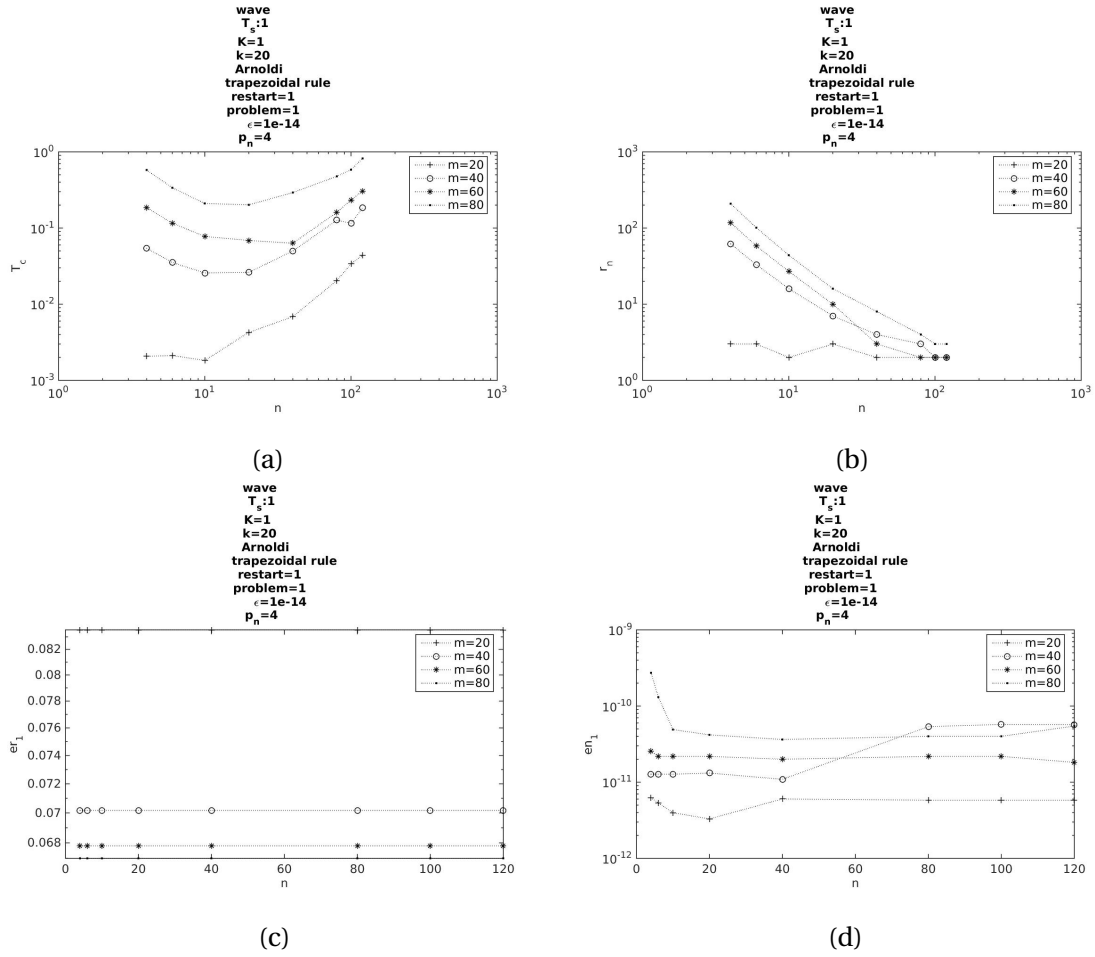
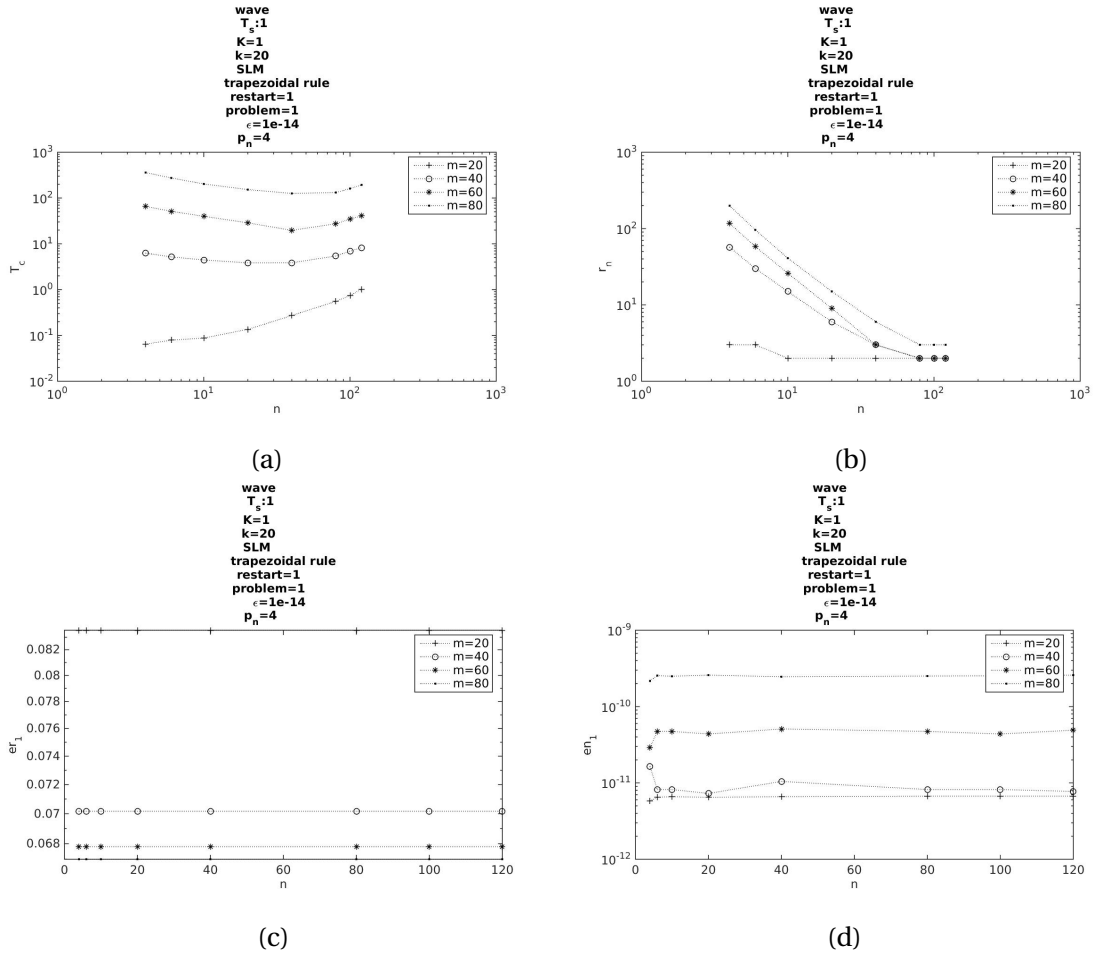


Figure 4.16: computation time, number of restarts, error and energy are all plotted here with different m and n.



(a) (b)

(c) (d)

Figure 4.17: computation time, number of restarts, error and energy are all plotted here with different m and n.

!!!!!!!!!!!!!!!Skriv noen commentarer her!!!!!!!!!!!!!!!!!!!!!!

4.7.2 Varying energy

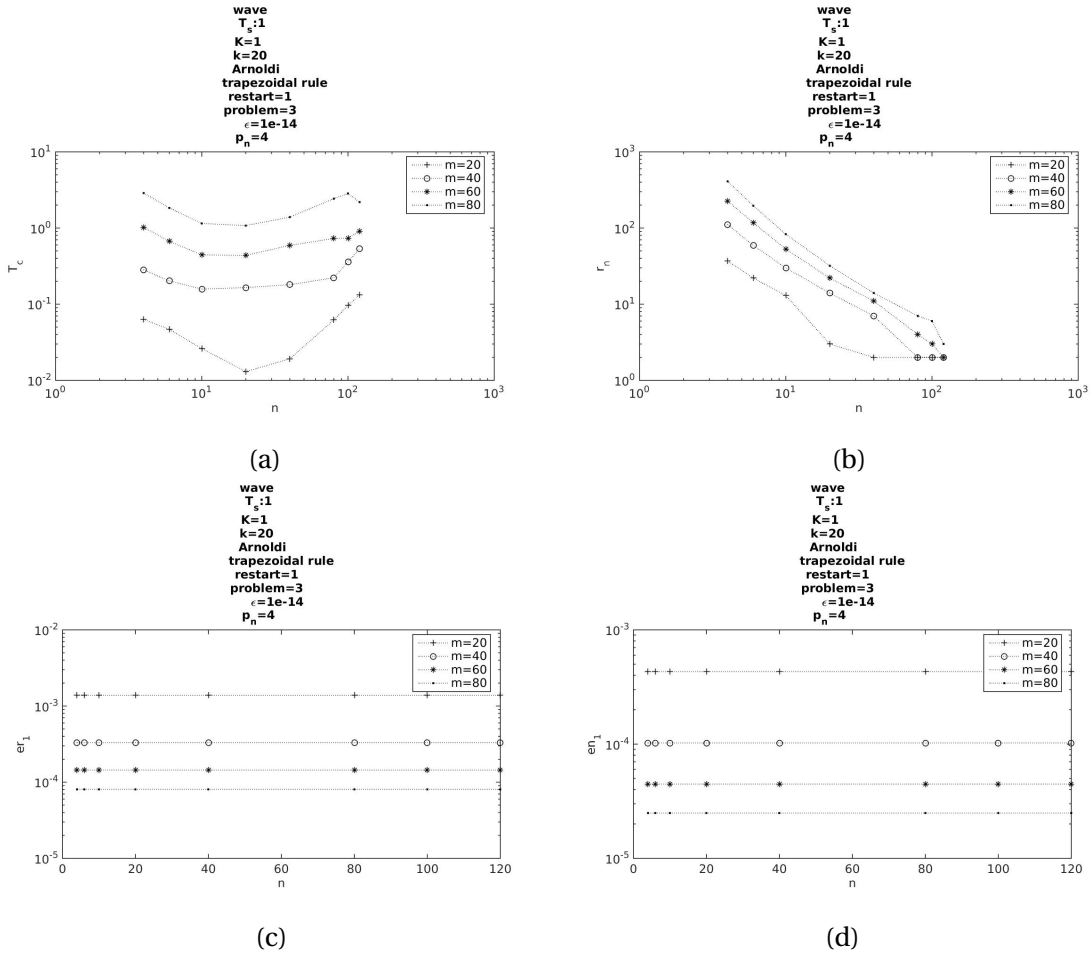


Figure 4.18: !!!!!!!!!!!!!!!!!SKRIV NOE HER!!!!!!!!!!!!!!!!!!

!!!!!!!!!!!!!!Kommentar her!!!!!!!!!!!!!

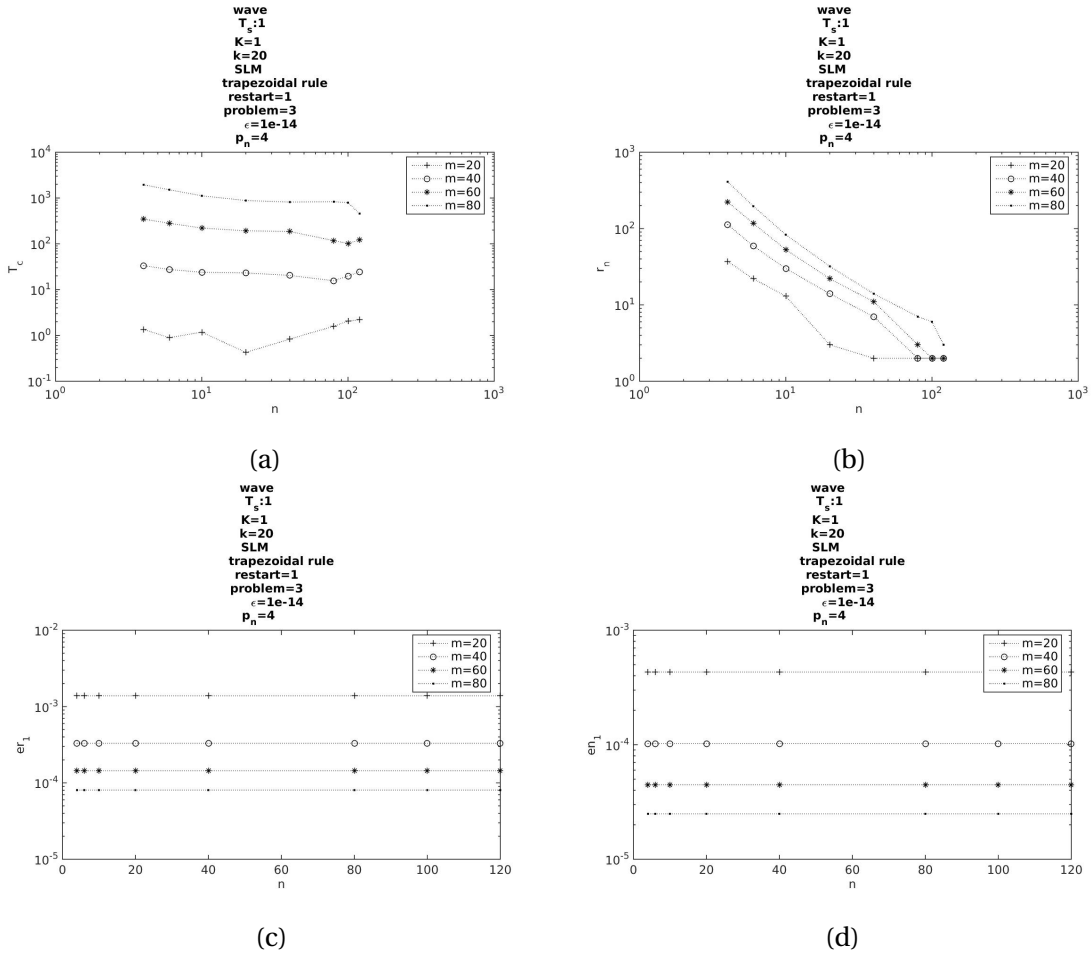


Figure 4.19: !!!!!!!!!!!!!!!!!SKRIV NOE HER!!!!!!!!!!!!!!!!!!!

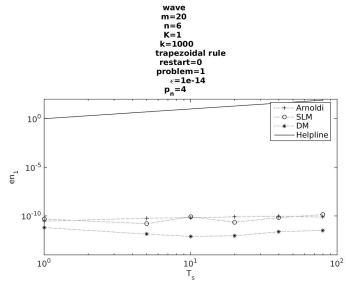
!!!!!!!!!!!!KOmmentar her!!!!!!!!!!!!!!!

figure 4.18 shows a few different important things. First figure 4.18c shows that the error and energy does not change (much) with n, only with m. The second thing is that the number of iterations needed to converge decreases when n becomes larger. The finale thing is that there seams to be a restart variable smaller than the dimension of A, and larger than one that is optimal. !!!!!!!!!!!!KOmmentar om forskjellene på Arnoldi og SLM!!!!!!!!!!!!!!!

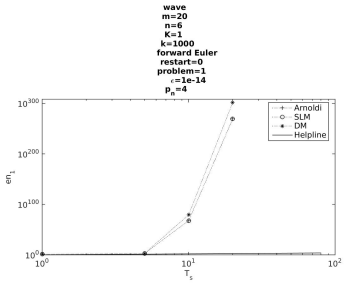
4.8 Integrating over looong time

This section will show how the energy changes when T_s increases, with everything else constant.

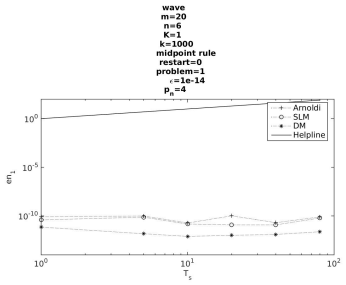
4.8.1 Constant energy



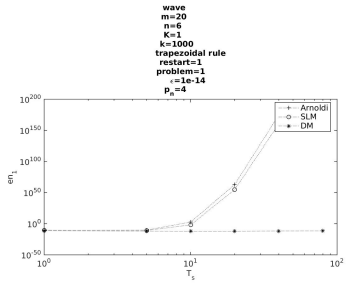
(a) Trapezoidal rule without restart. Helpline increases with T_s



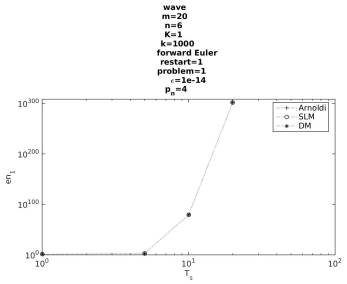
(b) Forward Euler without restart. Helpline increases with T_s^2



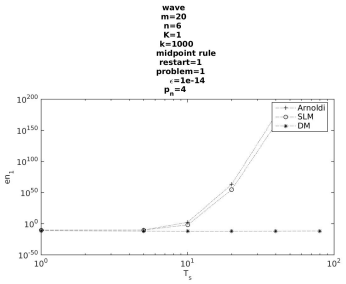
(c) Midpoint rule without restart. Helpline increases with T_s



(d) Trapezoidal rule with restart.



(e) Forward Euler with restart.

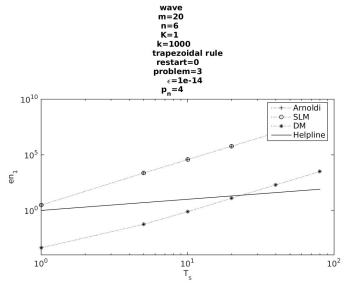


(f) Midpoint rule with restart.

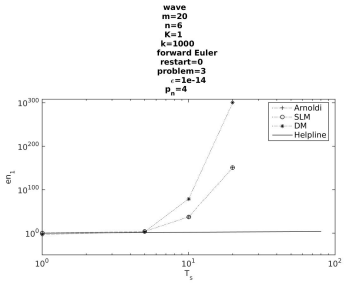
Figure 4.20: The figures shows how the energy for the different methods change with the different integration methods, with and without restart.

Without restart the energy for trapezoidal and midpoint rule increases linearly, while forward Euler's energy increases extremely fast. With restart the energy for all methods except DM increases very fast. The restart must be blamed for this, since it did not increase so fast when restart was not enabled. I would suspect that a larger increase in energy makes Arnoldi and SLM restart more, and more restarts add up to a larger energy, giving a feedback loop of diverging energy.

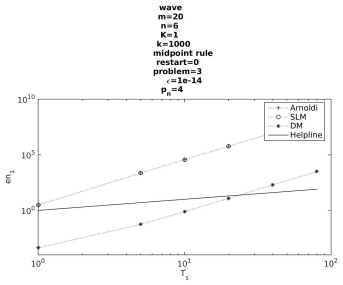
4.8.2 Varying energy



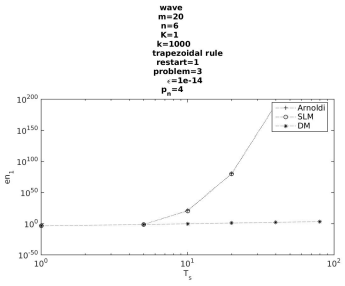
(a) Trapezoidal rule without restart. Helpline increases with T_s



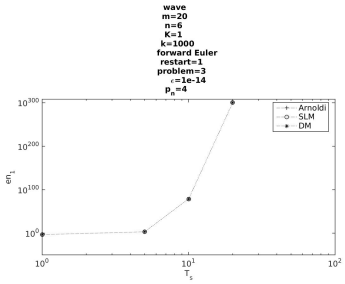
(b) Forward Euler without restart. Helpline increases with T_s^2



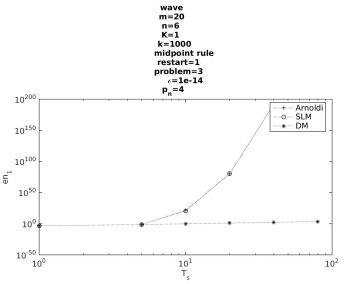
(c) Midpoint rule without restart. Helpline increases with T_s



(d) Trapezoidal rule with restart.



(e) Forward Euler with restart.



(f) Midpoint rule with restart.

Figure 4.21: The figures shows how the energy for the different methods change with the different integration methods, with and without restart.

The difference between constant energy and varying energy is again not huge. The energy increases faster for trapezidal rule and midpoint rule in this case, but apart from that it seams to be the same.

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