GENERALIZED NEWMARK ALGORITHMS

I – Newmark Method for second order (Hyperbolic) Equations

We start with the one-degree-of-fredom dynamic equation

$$\mathrm{m}\frac{d^2x}{dt^2} + F(x,\dot{x}) = g(x)\,,\quad x(0) = x_0\,,\quad \dot{x}(0) = \dot{x}_0$$

Here x is a "generalized" displacement. It can be temperature, velocity, concentration, etc. $\dot{x}$ and $\ddot{x}$ are "generalized" velocity and acceleration.

Suppose that x_n, $\dot{x}_n$ and $\ddot{x}_n$ are known at time $t = t_n$. We can approximate their values at time $t_{n+1} = t_n + \Delta t$ using Taylor series expansions for the displacement and velocity

$$x^{n+1} = x^n + \Delta t\,\dot{x}^n + \frac{(\Delta t)^2}{2}\left[(1-2\beta)\ddot{x}^n + 2\beta\ddot{x}^{n+1}\right]$$

$$\dot{x}^{n+1} = \dot{x}^n + \Delta t\left[(1-\gamma)\ddot{x}^n + \gamma\ddot{x}^{n+1}\right]$$

The parameters β and γ were introduced to include the acceleration $\ddot{x}^{n+1}$ implicitly in the numerical scheme, so that the forces at the end of the time step can be included to increase the accuracy of the method.

To develop the algorithm let us first assume that the function $F(x,\dot{x})$ is linear. So without loss of generality we can write

$$m\ddot{x} + \alpha\dot{x} + ax = g$$

where α, a, and g may be functions of time.

We write $x^{n+1} = p + \beta(\Delta t)^2\,\ddot{x}^{n+1}$ and $\dot{x}^{n+1} = \dot{p} + \gamma\,\Delta t\,\ddot{x}^{n+1}$

Where p and $\dot{p}$ are "predictors" defined as

$$p = x^n + \Delta t\,\dot{x}^n + \frac{1}{2}(1-2\beta)(\Delta t)^2\,\ddot{x}^n$$

$$\dot{p} = \dot{x}^n + \Delta t(1-\gamma)\ddot{x}^n$$

and are known at $t = t_n$.

Our goal is to find x^{n+1}, $\dot{x}^{n+1}$ and $\ddot{x}^{n+1}$ such that

$$m\ddot{x}^{n+1} + \alpha\dot{x}^{n+1} + ax^{n+1} = g^{n+1}$$

Substituting $x^{n+1} = p + \beta(\Delta t)^2\,\ddot{x}^{n+1}$ and $\dot{x}^{n+1} = \dot{p} + \gamma\,\Delta t\,\ddot{x}^{n+1}$ into $m\ddot{x}^{n+1} + \alpha\dot{x}^{n+1} + ax^{n+1} = g^{n+1}$, and setting $\Delta p = x^{n+1} - p$ we get

$$\left(\frac{\mathrm{m}}{\beta(\Delta t)^2} + \frac{\alpha\gamma}{\beta\Delta t} + a\right)\Delta p = g^{n+1} - \alpha\,\dot{p} - ap$$

This equation s solved for Δp, and then

$$x^{n+1} = x^n + \Delta p,\qquad \ddot{x}^{n+1} = \frac{x^{n+1} - p}{\beta(\Delta t)^2},\qquad \dot{x}^{n+1} = \dot{p} + \gamma\Delta t\ddot{x}^{n+1}$$

EXAMPLE

$$\frac{d^2x}{dt^2} - x = 0,\qquad x(0) = 1,\qquad \dot{x}(0) = 0,\qquad x^*(t) = \cosh(t)$$

We set $\beta = 1/4$, $\gamma = 1/2$ (these choices are dicussed later) and $\Delta t = 0.1$

$$p = x^n + \Delta t\,\dot{x}^n + \frac{1}{2}(1-2\beta)(\Delta t)^2\,\ddot{x}^n = x^0 + 0.1\dot{x}^0 + 0.0025\ddot{x}^0 = 1.0025$$

$$\dot{p} = \dot{x}^n + \Delta t(1-\gamma)\ddot{x}^n = \dot{x}^0 + 0.05\ddot{x}^0 = 0.05$$

Where we have used $x^0 = 1$, $\dot{x}^0 = 0$ and $\ddot{x}^0 = 1$

The equation becomes $\left(\frac{m}{\beta(\Delta t)^2} + a\right)\Delta p = 399\Delta p = -ap = 1.0025$ and from here $\Delta p = 0.0025125$. The solution is

	Calculated	Exact
x^1	1.005013	1.005005
$\dot{x}^1$	0.100251	0.100167
$\ddot{x}^1$	1.005013	1.005005

Here we have cheated because we used the exact solution to get a value for $\ddot{x}^0$. We need a starting value for $\ddot{x}^0$ but this is not part of the data. In practise we usually estimate an initial value from

$$\ddot{x}^0 = \frac{1}{m}\left[g - F\left(x^0, \dot{x}^0\right)\right]$$

For no-linear equations the Newmark method is combined with a Newton-Raphson iteration at each time step. The same steps are Followed with the Linearized Operator

The linearized operator for $\mathrm{m}\frac{d^2x}{dt^2} + F(x,\dot{x}) = g(x)$ is

$m\ddot{x} + c(x^{(i)},\dot{x}^{(i)})\dot{x} + k(x^{(i)},\dot{x}^{(i)})x$ where $x^{(i)}$ and $\dot{x}^{(i)}$ are the latest known approximations to x and $\dot{x}$, and

$$c(x,\dot{x}) = \frac{\partial F}{\partial \dot{x}}\quad\text{and}\quad \mathrm{k}(x,\dot{x}) = \frac{\partial F}{\partial x}$$

ALGORITHM:

1) Set $i = 0$ and construct the predictors $p_i, \dot{p}_i, \ddot{p}_i$

$$p_0 = x^n + \Delta t\,\dot{x}^n + \frac{1}{2}(1-2\beta)(\Delta t)^2\,\ddot{x}^n,\quad \dot{p}_0 = \dot{x}^n + \Delta t(1-\gamma)\ddot{x}^n,\quad \ddot{p}_0 = 0$$

2) Substitute into $\mathrm{m}\frac{d^2x}{dt^2} + F(x,\dot{x}) = g(x)$ and calculate the "out of balance" or "RESIDUAL" vector $\Delta Q_i = g^{n+1} - F(p_i,\dot{p}_i) - m\ddot{p}_i$

3) Find Δp_i from $\left(\frac{\mathrm{m}}{\beta(\Delta t)^2} + \frac{\gamma}{\beta\Delta t}c(p_i,\dot{p}_i) + k(p_i,\dot{p}_i)\right)\Delta p_i = \Delta Q_i$

4) Find the correctors $\mathrm{p}_{i+1} = \mathrm{p}_i + \Delta\mathrm{p}_i$

$$\ddot{\mathrm{p}}_{i+1} = \frac{\mathrm{p}_{i+1} - p_0}{\beta(\Delta t)^2}$$

$$\dot{\mathrm{p}}_{i+1} = \dot{p}_0 + \gamma\,\Delta t\,\ddot{\mathrm{p}}_{i+1}$$

5) Set $i = i+1$ and go back to step 2 to calculate ΔQ_{i+1}

6) If $|\Delta \mathrm{Q}_{i+1}| < \varepsilon$, a predetermined tolerance, then set $x^{n+1} = p_{i+1}$, $\dot{x}^{n+1} = \dot{p}_{i+1}$, $\ddot{x}^{n+1} = \ddot{p}_{i+1}$, and the time step is completed. Otherwise go back to step 3) and complete the next iteration.

EXAMPLE

$$\frac{d^2x}{dt^2}-\frac{x}{t}\frac{dx}{dt}=0,\quad x(1)=-1,\quad \dot{x}(1)=2,\quad x^*(t)=2\tan(\ln t)-1$$

Set $\ddot{x}(1)=-2,\ \beta=1/4,\ \gamma=1/2,\ \varepsilon=10^{-8}$, and $\Delta t=0.1$

The linearized functions are $c(x,\dot{x})=-\frac{x}{t}$ and $k(x,\dot{x})=-\frac{\dot{x}}{t}$,
and for $i=0$ we have $p_0=-0.805,\ \dot{p}_0=1.9,\ \ddot{p}_0=0.0$

1. First iteration, $i=0$: $\Delta Q_0=-F(p_0,\dot{p}_0)=\frac{p_0\dot{p}_0}{t_1}=-1.39045$

$$\left(\frac{m}{\beta(\Delta t)^2}+\frac{\gamma}{\beta\Delta t}\left(-\frac{p_0}{t_1}\right)+\left(-\frac{\dot{p}_0}{t_1}\right)\right)\Delta p_0=\Delta Q_0$$

$$(400+20(-0.73181)+(-1.72723))\Delta p_0=-1.39045\ \Rightarrow \Delta p_0=-0.00336746$$

$$p_1=-0.808367459,\ \dot{p}_1=1.832650815,\ \ddot{p}_1=-1.346983707$$

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2. Second iteration $i=1$, $\Delta Q_1=\frac{p_1\dot{p}_1}{t_1}-m\ddot{p}_1=0.000206177$

$$\Delta p_1=\Delta Q_1\Big/\left(\frac{m}{\beta(\Delta t_1)^2}-\frac{\gamma p_1}{t_1\beta\Delta t_1}-\frac{\dot{p}_1}{t_1}\right)=0.000000499$$

$p_2=-0.80836696,\ \dot{p}_2=1.832660799,\ \ddot{p}_2=-1.34678404$

3. Third iteration, $i=2$, $\Delta Q_2=\frac{p_2\dot{p}_2}{t_2}-m\ddot{p}_2=5\times10^{-9}<\varepsilon$ STOP

	Calculated	Exact
x_1	−0.808367	−0.808800
$\dot{x}_1$	1.832661	1.834799
$\ddot{x}_1$	−1.346784	−1.349078

SYSTEMS OF (NON-LINEAR) HYPERBOLIC EQUATIONS

$$\mathbf{M}\ddot{\boldsymbol{\varphi}}+\mathbf{N}(\boldsymbol{\varphi},\dot{\boldsymbol{\varphi}})=\mathbf{F}$$

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General Algorithm

1) Predictors, $i=0$: $\mathbf{p}^0=\boldsymbol{\varphi}_n+\Delta t\dot{\boldsymbol{\varphi}}_n+\frac{(\Delta t)^2}{2}(1-2\beta)\ddot{\boldsymbol{\varphi}}_n$

$$\dot{\mathbf{p}}^0=\dot{\boldsymbol{\varphi}}_n+\Delta t(1-\gamma)\ddot{\boldsymbol{\varphi}}_n$$

$$\ddot{\mathbf{p}}^0=\mathbf{0}$$

2) Calculate the residual vector $\Delta\mathbf{Q}^i=\mathbf{F}(t_{n+1})-\mathbf{N}(\mathbf{p}^i,\dot{\mathbf{p}}^i)-\mathbf{M}\ddot{\mathbf{p}}^i$

3) Calculate the tangent matrices $\mathbf{C}=\frac{\partial\mathbf{N}}{\partial\dot{\mathbf{p}}},\ \left[c_{ij}\right]=\left[\frac{\partial N_i}{\partial\dot{p}_j}\right]$

$$\mathbf{K}=\frac{\partial\mathbf{N}}{\partial\mathbf{p}},\ \left[k_{ij}\right]=\left[\frac{\partial N_i}{\partial p_j}\right]$$

4) Solve for $\Delta\mathbf{p}^i$: $\left[\frac{1}{\beta(\Delta t)^2}\mathbf{M}+\frac{\gamma}{\beta\Delta t}\mathbf{C}(\mathbf{p}^i,\dot{\mathbf{p}}^i)+\mathbf{K}(\mathbf{p}^i,\dot{\mathbf{p}}^i)\right]\Delta\mathbf{p}^i=\Delta\mathbf{Q}^i$

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5) Correctors: $\mathbf{p}^{i+1}=\mathbf{p}^i+\Delta\mathbf{p}^i$

$$\ddot{\mathbf{p}}^{i+1}=\frac{1}{\beta(\Delta t)^2}\left(\mathbf{p}^i-\mathbf{p}^0\right)$$

$$\dot{\mathbf{p}}^{i+1}=\dot{\mathbf{p}}^0+\gamma\Delta t\,\ddot{\mathbf{p}}^{i+1}$$

6) Go to step 2) and calculate $\Delta\mathbf{Q}^{i+1}=\mathbf{F}(t_{n+1})-\mathbf{N}(\mathbf{p}^{i+1},\dot{\mathbf{p}}^{i+1})-\mathbf{M}\ddot{\mathbf{p}}^{i+1}$

7) Check convergence:

a) If $\left\|\Delta\mathbf{Q}^{i+1}\right\|<\varepsilon$ then $\boldsymbol{\varphi}^{n+1}=\mathbf{p}^{i+1}$, $\dot{\boldsymbol{\varphi}}^{n+1}=\dot{\mathbf{p}}^{i+1}$, $\ddot{\boldsymbol{\varphi}}^{n+1}=\ddot{\mathbf{p}}^{i+1}$

b) If $\left\|\Delta\mathbf{Q}^{i+1}\right\|>\varepsilon$ then set $i=i+1$ and continue with step 3)

REMARKS:

1) The convergence test in step 7) is the most appropriate. The norms usually used are Euclidean $\left\|\Delta\mathbf{Q}\right\|_E=\left(\sum_k(\Delta Q_k)^2\right)^{1/2}$ and the maximum norm $\left\|\Delta\mathbf{Q}\right\|_M=\max_k\left|\Delta Q_k\right|$

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2) The matrices **C** and **K** are normally evaluated only once at the start of the iteration (i = 0) to save CPU time.

EXAMPLE

$$\frac{\partial^2u}{\partial t^2}-\frac{\partial^2u}{\partial x^2}-\sin(u)=0,\ \left(\frac{\partial u}{\partial x}\right)_{x=a}=\left(\frac{\partial u}{\partial x}\right)_{x=b},\ u(x,0)=f(x),\ \dot{u}(x,0)=g(x)$$

Because the aproximation $\sin(u)\cong\sin\left(\sum_i N_i(x)u_i\right)$ is not practical, we introduce the "*PRODUCT APPROXIMATION*"

$$\sin(u)\cong\sum_i N_i(x)\sin(u_i)$$

It has been proved that this approximations do not cause loss of accuracy in a variety of situations. However a general proof is not available and its appropriate ness must be checked case by case. The element equations become:

$$\frac{h}{6}\begin{bmatrix}2&1\\1&2\end{bmatrix}\begin{bmatrix}\ddot{u}_1\\\ddot{u}_2\end{bmatrix}+\frac{1}{h}\begin{bmatrix}1&-1\\-1&1\end{bmatrix}\begin{bmatrix}u_1\\u_2\end{bmatrix}-\frac{h}{6}\begin{bmatrix}2\sin u_1+\sin u_2\\\sin u_1+2\sin u_2\end{bmatrix}=\begin{bmatrix}0\\0\end{bmatrix}$$

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Predictors: $\mathbf{p}^0=\begin{bmatrix}p_1^0\\p_2^0\end{bmatrix}=\begin{bmatrix}u_1^n+\frac{1}{2}(1-2\beta)(\Delta t)^2\ddot{u}_1^0\\u_2^n+\frac{1}{2}(1-2\beta)(\Delta t)^2\ddot{u}_2^0\end{bmatrix}$, $\ddot{\mathbf{p}}^0=\begin{bmatrix}0\\0\end{bmatrix}$

Tangent matrices: $\mathbf{C}=\mathbf{0}$, $\mathbf{K}=\begin{bmatrix}\frac{1}{h}-\frac{h}{3}\cos u_1&-\frac{1}{h}-\frac{h}{6}\cos u_2\\-\frac{1}{h}-\frac{h}{6}\cos u_1&\frac{1}{h}-\frac{h}{3}\cos u_2\end{bmatrix}$

Out of balance vector

$$\Delta\mathbf{Q}^i=\frac{h}{6}\begin{bmatrix}2\sin p_1^i+\sin p_2^i\\\sin p_1^i+2\sin p_2^i\end{bmatrix}-\frac{1}{h}\begin{bmatrix}p_1^i-p_2^i\\p_2^i-p_1^i\end{bmatrix}-\frac{h}{6}\begin{bmatrix}2\ddot{p}_1^i+\ddot{p}_2^i\\\ddot{p}_1^i+2\ddot{p}_2^i\end{bmatrix}$$

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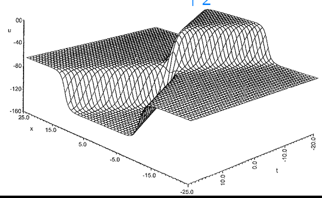
Element equations for $\Delta \mathbf{p}^i$

$$\left\{ \frac{h}{6\beta(\Delta t)^2} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} + \begin{bmatrix} \frac{1}{h} - \frac{h}{3}\cos u_1 & -\frac{1}{h} - \frac{h}{6}\cos u_2 \\ -\frac{1}{h} - \frac{h}{6}\cos u_1 & \frac{1}{h} - \frac{h}{3}\cos u_2 \end{bmatrix} \right\} \begin{bmatrix} \Delta p_1^i \\ \Delta p_2^i \end{bmatrix} = \Delta \mathbf{Q}^i$$

Because there is no first derivative the parameter γ is not needed

Solution for $-25 \le x \le 25$, $t_0 = -20 \le t \le 20$ and $f(x)$, $g(x)$ chosen so that the exact solution is $u(x,t) = 4\tan^{-1}\left[\frac{1}{2}\cosh(1.1547x)\operatorname{cosech}(0.57735t)\right]$



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ACCURACY AND STABILITY

If $\gamma \ge 1/2$ the method is unconditionally stable in the linearized sense, as long as $\beta \ge \gamma/2$. If $\beta < \gamma/2$ stability is conditional. Moreover, the value $\beta = \frac{1}{4}\left(\gamma + \frac{1}{2}\right)^2$ maximizes the high frequency numerical dissipation.

As was the case for the θ-method, when γ=1/2 the scheme is second order accurate in time. For γ>1/2 in general accuracy is only first order .

This is why the values β=1/4 and γ=1/2 are the most frequently used.

II – Generalized Newmark Method for first order (Parabolic) Equations

$$\frac{\partial \phi}{\partial t} + N(\phi) = f(t)$$

The variables ϕ and $\dot{\phi}$ are treated as generalized velocity and acceleration respectively. Therefore, since there is no equivalent to displacement, the β parameter is not needed.

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1) Predictors, i=0 $\quad \mathrm{p}^0 = \phi^n + (1-\gamma)\Delta t \dot{\phi}^n$, $\quad \dot{\mathrm{p}}^0 = 0$

2) Out of balance force $\quad \Delta \mathrm{Q}^i = f_{n+1} - N(p^i) - \dot{p}_i$

3) Linearized operator $\quad \mathrm{A}(\mathrm{p}_i) = \frac{1}{\gamma \Delta t} + k(p_i), \quad k(\phi) = \frac{\partial f}{\partial \phi}$

4) Solve $\quad \Delta \mathrm{p}^i = \frac{\Delta Q^i}{A(p^i)}$

5) Correctors $\quad \mathrm{p}^{i+1} = \mathrm{p}^i + \Delta \mathrm{p}^i$

$$\dot{\mathrm{p}}^{i+1} = \frac{\mathrm{p}^{i+1} - \mathrm{p}^0}{\gamma \Delta t}$$

It is easy to show that if the equation is linear, the algorithm is identical to the θ – method. This provides an extension of the θ – method to non-linear equations.

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SYSTEMS DERIVED FROM SEMI-DISCRETE GALERKIN FEM APPROXIMATIONS

$$\mathbf{C}\dot{\boldsymbol{\varphi}} + \mathbf{N}(\boldsymbol{\varphi}) = \mathbf{F}$$

1) Predictors $\quad \mathbf{p}^0 = \boldsymbol{\varphi}^n + (1-\gamma)\Delta t \dot{\boldsymbol{\varphi}}^n$, $\quad \dot{\mathbf{p}}^0 = \mathbf{0}$

2) Out of balance vector $\quad \Delta \mathbf{Q}^i = \mathbf{F}_{n+1} - \mathbf{N}(\mathbf{p}^i) - \mathbf{C}\dot{\mathbf{p}}^i$

3) Tangent operator $\quad \mathbf{K} = \frac{\partial \mathbf{N}}{\partial \mathbf{p}} \quad \left[k_{ij}\right] = \left[\frac{\partial N_i}{\partial p_j}\right]$

4) Find $\Delta \mathbf{p}^i$ from $\quad \left[\frac{1}{\gamma \Delta t}\mathbf{C} + \mathbf{K}(\mathbf{p}^i)\right]\Delta \mathbf{p}^i = \Delta \mathbf{Q}^i$

5) Correctors $\quad \mathbf{p}^{i+1} = \mathbf{p}^i + \Delta \mathbf{p}^i, \quad \dot{\mathbf{p}}^{i+1} = \frac{1}{\gamma \Delta t}\left(\mathbf{p}^i - \mathbf{p}^0\right)$

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Example

Solve the Burgers equation with ε = 1 using 4 Linear elements.

$$\frac{\partial u}{\partial t} u \frac{\partial u}{\partial x} = \varepsilon \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < 1, \quad u(0,t) = 1, \ u(1,t) = 0), \quad u(x,0) = \begin{cases} 1 \ if \ \ x \le \frac{1}{4} \\ 0 \ if \ \ x > \frac{1}{4} \end{cases}$$

$$\mathbf{C}\dot{\mathbf{u}} + \mathbf{N}(\mathbf{u}) = \frac{1}{24}\begin{bmatrix} 4 & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & 4 \end{bmatrix}\begin{bmatrix} \dot{u}_2 \\ \dot{u}_3 \\ \dot{u}_4 \end{bmatrix} + \begin{bmatrix} 8u_2 - 4u_3 - \frac{1}{6}u_2 + \frac{1}{6}u_2u_3 + \frac{1}{6}u_3^2 - \frac{1}{6} \\ -4u_2 + 8u_3 - 4u_4 - \frac{1}{6}u_2^2 - \frac{1}{6}u_2u_3 + \frac{1}{6}u_3u_4 + \frac{1}{6}u_4^2 \\ -4u_3 + 8u_4 - \frac{1}{6}u_3^2 - \frac{1}{6}u_3u_4 \end{bmatrix} = \mathbf{0}$$

$$\Delta \mathbf{Q}^i = \begin{bmatrix} 8p_2^i - 4p_3^i - \frac{1}{6}p_2^i + \frac{1}{6}p_2^ip_3^i + \frac{1}{6}\left(p_3^i\right)^2 - \frac{1}{6} \\ -4p_2^i + 8p_3^i - 4p_4^i - \frac{1}{6}\left(p_2^i\right)^2 - \frac{1}{6}p_2^ip_3^i + \frac{1}{6}p_3^ip_4^i + \frac{1}{6}\left(p_4^i\right)^2 \\ -4p_3^i + 8p_4^i - \frac{1}{6}\left(p_3^i\right)^2 + \frac{1}{6}p_3^ip_4^i \end{bmatrix} - \frac{1}{24}\begin{bmatrix} 4\dot{p}_2^i + \dot{p}_3^i \\ \dot{p}_2^i + 4\dot{p}_3^i + \dot{p}_4^i \\ \dot{p}_3^i + 4\dot{p}_4^i \end{bmatrix}$$

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$$\mathbf{K} = \begin{bmatrix} 8 - \frac{1}{6}u_2 + \frac{1}{6}u_3 & -4 + \frac{1}{6}u_2 + \frac{1}{3}u_3 & 0 \\ -4 - \frac{1}{3}u_2 - \frac{1}{6}u_3 & 8 - \frac{1}{6}u_2 + \frac{1}{6}u_4 & -4 + \frac{1}{6}u_3 + \frac{1}{3}u_4 \\ 0 & -4 - \frac{1}{3}u_3 - \frac{1}{6}u_4 & 8 - \frac{1}{6}u_3 \end{bmatrix}$$

Tangent Matrix

Increment equations

$$\left\{ \frac{1}{\gamma \Delta t}\begin{bmatrix} 4 & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & 4 \end{bmatrix} + \begin{bmatrix} 8 - \frac{1}{6}p_2^i + \frac{1}{6}p_3^i & -4 + \frac{1}{6}p_2^i + \frac{1}{3}p_3^i & 0 \\ -4 - \frac{1}{3}p_2^i - \frac{1}{6}p_3^i & 8 - \frac{1}{6}p_2^i + \frac{1}{6}p_4^i & -4 + \frac{1}{6}p_3^i + \frac{1}{3}p_4^i \\ 0 & -4 - \frac{1}{3}p_3^i - \frac{1}{6}p_4^i & 8 - \frac{1}{6}p_3^i \end{bmatrix} \right\} \Delta \mathbf{p}^i = \Delta \mathbf{Q}^i$$

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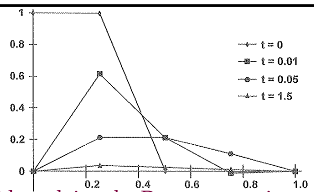
Solution with

$\gamma = 1/2$ and $\Delta t = 0.005$



As a final example, consider solving the Burgers equation with boundary conditions $u(0,t) = 1,\ u(1,t) = 0$ and initial condition u(x,0)=0. The analytical solution at steady-state is well known. We also choose $\varepsilon = \Delta x = \Delta t = 0.1$. The steady state results are

x	Finite element solution	Analytical solution
0.0	1.000	1.000
0.2	1.000	0.999
0.4	0.997	0.995
0.6	0.970	0.964
0.8	0.770	0.762
0.9	0.464	0.462
1.0	0.000	0.000

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Now set ε=0.01 keeping the rest of the problem unchanged. We get

x	Finite element solution	Analytical solution
0.0	1.000	1.000
0.1	1.032	1.000
0.2	0.985	1.000
0.3	1.057	1.000
0.4	0.945	1.000
0.5	1.101	1.000
0.6	0.854	1.000
0.7	1.213	1.000
0.8	0.648	1.000
0.9	1.457	1.000
1.0	0.000	0.000

We observe an oscillatory solution. This is not an error, it is the Solution we will obtain with any kind of discretization that does Not take special measures to account for the fact that the equation Has become "CONVECTION DOMINATED".

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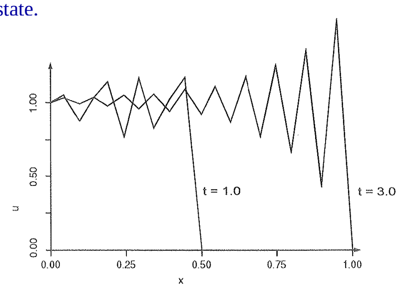
Further illustration:

Below we show the solution when $\varepsilon = 0.0025,\ \Delta x = 0.5,\ \Delta t = 0.05$. The figure shows the solution at $t = 1.0$, when the wave has advanced halfway into the domain, and at time $t = 3.0$ which is essentially steady-state.



We now address the solution to these difficulties.

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STEADY-STATE CONVECTIVE TRANSPORT

Let us start with the model equation for one-dimensional convection-diffusion

$$-\frac{d}{dx}\left(D\frac{d\phi}{dx}\right) + u\frac{d\phi}{dx} = 0$$

The character of the equation changes from that of an elliptic boundary value problem to that of a first order hyperbolic initial value problem according to the value of D/u

Even when D/u << 1 there will be regions where the second order curvature dominates. We usually refer to these regions as Boundary Layers.

The weighted residual form is

$$\int_0^L \left(D\frac{dw}{dx}\frac{d\phi}{dx} + wu\frac{d\phi}{dx} \right) dx + \left[w\left(-D\frac{d\phi}{dx} \right) \right]_{x=0}^{x=L} = 0$$

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Discretize using Linear elements of size $\Delta x = h$ and apply the Galerkin method. The element stiffness matrix becomes

$$\mathbf{k}_e = \begin{bmatrix} \frac{D}{h} - \frac{u}{2} & -\frac{D}{h} + \frac{u}{2} \\ -\frac{D}{h} - \frac{u}{2} & \frac{D}{h} + \frac{u}{2} \end{bmatrix}$$

The Global, assembled stiffness matrix becomes

$$\mathbf{K} = \begin{bmatrix} \frac{D}{h} - \frac{u}{2} & -\frac{D}{h} + \frac{u}{2} & 0 & 0 & \dots & 0 & 0 & 0 \\ -\frac{D}{h} - \frac{u}{2} & \frac{2D}{h} & -\frac{D}{h} + \frac{u}{2} & 0 & \dots & 0 & 0 & 0 \\ 0 & -\frac{D}{h} - \frac{u}{2} & \frac{2D}{h} & -\frac{D}{h} + \frac{u}{2} & \dots & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & -\frac{D}{h} - \frac{u}{2} & \frac{2D}{h} & -\frac{D}{h} + \frac{u}{2} \\ 0 & 0 & 0 & 0 & \dots & 0 & -\frac{D}{h} - \frac{u}{2} & \frac{D}{h} + \frac{u}{2} \end{bmatrix}$$

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K differs in two important ways from the matrices we obtained before for heat conduction:
1) It is NOT SYMMETRIC
2) As D/u $\ll 1$, the matrix is no longer diagonally dominant.

Different analysis tools are needed to understand the behavior. Look at a typical difference equation

$$\left(-\frac{D}{h} - \frac{u}{2}\right)\phi_{i-1} + \frac{2D}{h}\phi_i + \left(-\frac{D}{h} + \frac{u}{2}\right)\phi_{i+1} = 0 \quad \text{define } \gamma = \frac{uh}{D}$$

where γ is the local Peclet number. Re-writing the equation

$$\left(-1 - \gamma/2\right)\phi_{i-1} + 2\phi_i + \left(-1 + \gamma/2\right)\phi_{i+1} = 0$$

This has a solution of the form $\phi_i = \lambda^i$ where $\lambda_1 = 1$, $\lambda_2 = (2+\gamma)/(2-\gamma)$

that is $\quad \phi_i = A + B\left(\frac{2+\gamma}{2-\gamma}\right)^i \quad i = 1, 2, \dots, N$

A and B are determined from the boundary conditions.

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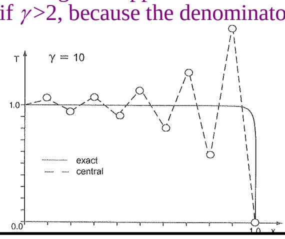
The exact solution to the differential equation is $\phi(x) = c_1 + c_2 e^{(u/D)x}$

Hence the discrete solution represents the exponential term as

$$e^{(u/D)x_i} = e^{\gamma \cdot i} \cong \left(\frac{2+\gamma}{2-\gamma}\right)^i + O(h^3)$$

where $x_i = (i-1)h$. This is called a (1,1) Pade$'$ rational approximation

Note that even though the approximation is $O(h^3)$, the solution is oscillatory if γ>2, because the denominator becomes negative.



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The error analysis yields $\left\|\phi^* - \phi^h\right\|_\infty = O(h^2)$. However, when $|\gamma|$ is large, the expresion $e^{(u/D)x_i} \cong \left(\frac{2+\gamma}{2-\gamma}\right)^i$ does not have the correct asymptotic behavior.

To illustrate this re-write the difference equation as

$\frac{1}{\gamma}(-\phi_{i-1} + 2\phi_i - \phi_{i+1}) + \frac{1}{2}(\phi_{i+1} - \phi_{i-1}) = 0$ and take the limit as $\gamma \to \infty$.

The difference equation reduces to $\phi_{i+1} = \phi_{i-1}$ a Leap-Frog solution.

If the mesh has an even number of nodes then the boundary condition at $x = L$ determines the value at all even nodes including x_2. However, if u>0 there is no physical mechanism to propagate perturbations in the backward direction.

When $\gamma \gg 1$ the mesh length is too large compared to the diffusion length scale. The Galerkin approximation to the convective term is $u\left.\frac{d\phi}{dx}\right|_{x=x_i} \cong \frac{u}{2}(\phi_{i+1} - \phi_{i-1})$ and the value at x_{i+1} affects what happens at x_i.

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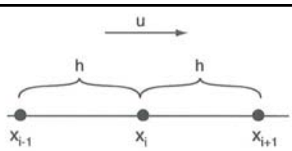

To avoid this non-physical behavior and make $\gamma < 2$ we can only make h smaller, but values of γ that are $O(10^4 - 10^9)$ are common. We need somethig better.

People that use finite differences introduced *Upwind Differences*

$$u\left.\frac{d\phi}{dx}\right|_{x=x_i} \cong \begin{cases} \frac{u}{h}(\phi_i - \phi_{i-1}) & if \quad u > 0 \\ \frac{u}{h}(\phi_i - \phi_{i+1}) & if \quad u < 0 \end{cases}$$

If u>0, this leads to difference equations of the form

$$-(1+\gamma)\phi_{i-1} + (2+\gamma)\phi_i - \phi_{i+1} = 0$$

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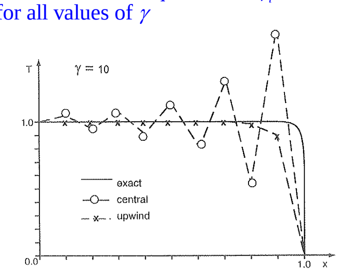
Note that now the matrix $\mathbf{K}$ is positive definite for all γ, and the solution to the difference equation is $\phi_i = A + B(1+\gamma)^i$ and this is stable for all values of γ



So upwinding appears to provide a simple solution. However, it turns out that the approximations are too inaccurate, as shown, unless h is unacceptably small.

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Let us perform a truncation error analysis on the difference equation written as $\frac{D}{h^2}(-\phi_{i-1} + 2\phi_i - \phi_{i+1}) + \frac{u}{h}(\phi_i - \phi_{i-1})$. Let $\phi_i^{(k)} \equiv \frac{d^k\phi}{dx^k}$ then

$$\phi_{i+1} = \phi_i + h\phi_i^{(1)} + \frac{h^2}{2}\phi_i^{(2)} + \frac{h^3}{3!}\phi_i^{(3)} + \frac{h^4}{4!}\phi_i^{(4)} + HOT$$

$$\phi_{i-1} = \phi_i - h\phi_i^{(1)} + \frac{h^2}{2}\phi_i^{(2)} - \frac{h^3}{3!}\phi_i^{(3)} + \frac{h^4}{4!}\phi_i^{(4)} + HOT$$

Then $\left(-\phi_{i-1} + 2\phi_i - \phi_{i+1}\right) = -h^2\phi_i^{(2)} - \frac{h^4}{12}\phi_i^{(4)} + HOT$ or

$$\left(-D\phi_i^{(2)}\right) - \frac{D}{h^2}\left(-\phi_{i-1} + 2\phi_i - \phi_{i+1}\right) = \frac{Dh^2}{12}\phi_i^{(4)} + HOT$$

Similarly $\phi_i - \phi_{i-1} = h\phi_i^{(1)} - \frac{h^2}{2}\phi_i^{(2)} + \frac{h^3}{6}\phi_i^{(3)} + HOT$, therefore

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$$u\phi_i^{(1)} - \frac{u}{h}(\phi_i - \phi_{i-1}) = \frac{uh}{2}\phi_i^{(2)} - \frac{uh^2}{6}\phi_i^{(3)} + HOT$$

Putting all together we have

$$\left(-D\frac{d^2\phi}{dx^2} + u\frac{d\phi}{dx}\right)_{x=x_i} - \left(\frac{D}{h^2}\left(-\phi_{i-1} + 2\phi_i - \phi_{i+1}\right)\right) =$$

$$\underbrace{\frac{uh}{2}\phi_i^{(2)} - \frac{h^2}{6}\left(u\phi_i^{(3)} + \frac{D}{2}\phi_i^{(4)}\right)}_{\text{Truncation error}} + HOT$$

There are two problems with the truncation error.

1) The leading term $\frac{uh}{2}\phi_i^{(2)}$ is only $O(h)$, linear we have lost the second order approximation.

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2) It contains $\phi_i^{(2)}$, so to interpret the approximation correctly we must move it to the left hand side and interpret the difference approximation as discretizing the equation

$$-\left(D+\frac{uh}{2}\right)\frac{d^2\phi}{dx^2}+u\frac{d\phi}{dx}=0$$

The term $\frac{uh}{2}$ is called *Artificial Numerical Diffusion* and in general is much larger than *D*. So we are solving a different problem.

Upwind differncing achieves stability by adding an artificial diffusion to the discretizd equation. Also, it can be shown by a slightly more involved analysis that the Galerkin method is "*underdiffused*" even with $\gamma < 2$.

This suggests that we should be able to find a method that is in-between upwind and Galerkin and that has zero numerical diffusion.