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# A TIME DISCONTINUOUS PETROV-GALERKIN METHOD FOR THE INTEGRATION OF INELASTIC CONSTITUTIVE EQUATIONS

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**Key words:** Implicit integration, discontinuous Galerkin method, Runge-Kutta method, creep, inelasticity, accuracy

**Abstract.** *A major task in computational inelasticity is the temporal integration of constitutive equations. In creep analysis, the time steps to be used in practical computations are often large, several magnitudes larger than the critical time step of some explicit method, e.g. the forward Euler method. Therefore the integrator should be unconditionally stable and sufficiently accurate for large time steps. The asymptotic convergence rate does not necessarily reflect high accuracy outside the asymptotic range, which is usually step sizes smaller than the critical time step of the explicit Euler method.*

*In this paper an approach based on time discontinuous Petrov-Galerkin type method is proposed. In a linear non-autonomous case, it reduces to the asymptotically second order accurate Lobatto IIIC type implicit Runge-Kutta method, which is equal to the Padé-(0,2) approximation of the exponential function. Within this approach it is possible to design an algorithm which yields asymptotically third order accurate scheme, the dG(1) method, without loosing accuracy in the large time step regime.*

*Accuracy and efficiency of the proposed method is studied in detail for viscoplastic and creep models. Comparison is made to the commonly used backward Euler method which gives accurate results for large time steps.*

## 1 INTRODUCTION

There are many different algorithms for the integration of inelastic constitutive models. However, the fully implicit backward Euler scheme seems to be the most popular one, although it is asymptotically only first order accurate [1, 2, 3].

In analysing practical problems, the time steps to be used are often large, several magnitudes larger than the critical time step of some explicit method, e.g. the forward Euler method. Therefore the integrator should be unconditionally stable and sufficiently accurate for large time steps. As shown in ref. [4] the asymptotic convergence rate does not necessarily reflect high accuracy outside the asymptotic range, which is usually step sizes smaller than the critical time step of the explicit Euler method. Asymptotically first order accurate implicit Euler method seems to be more accurate than many asymptotically higher order schemes for large time-steps [4].

Second order accurate two-stage Lobatto IIIC type implicit Runge-Kutta method (IRKL3C) exhibits good accuracy properties also for large time-steps. In this study a discontinuous Petrov-Galerkin type integrataror is developed which has similar properties than the IRKL3C-method.

## 2 SCALAR MODEL PROBLEM

As a simple uniaxial model problem, a Maxwell type creep model is considered. In Maxwell's model the inelastic strain rate is defined as $\dot{\epsilon}^{\text{in}} = \gamma(\sigma/\sigma_{\text{ref}})$, where $\gamma$ is the viscosity parameter and $\sigma_{\text{ref}}$ is a reference stress. Resulting evolution equation for the stress is

$$\dot{\sigma} + (E\gamma/\sigma_{\text{ref}})\sigma = E\dot{\epsilon} \tag{1}$$

where $E$ is the Young's modulus and $\dot{\epsilon}$ is the total strain rate. Therefore, a simple scalar constant coefficient evolution equation ($\sigma$ replaced by the symbol $y$ and $\sigma_{\text{ref}}$ by $y_{\text{ref}}$, respectively)

$$\dot{y} + \lambda y = f, \qquad y(0) = y_0 \tag{2}$$

will be considered ($\lambda = E\gamma/\sigma_{\text{ref}} \geq 0$). In view of equation (1) and (2) and the integration of a material model in a finite element software, a constant "forcing" term is present, therefore it can be expressed in a form

$$f = \eta\lambda y_{\text{ref}} \tag{3}$$

where $\eta = \dot{\epsilon}/\gamma$ is a nondimensional parameter.

For constant $\lambda$, the problem (2) has a simple analytical solution

$$y(t) = y_{\text{ref}} \left[ \left( \frac{y_0}{y_{\text{ref}}} - \eta \right) \exp(-\lambda t) + \eta \right] \tag{4}$$

Notice, that $y(t) \longrightarrow \eta y_{\text{ref}}$ when $t \longrightarrow \infty$.

## 3 NUMERICAL INTEGRATION

In this section the basic equations of discontinuous Galerkin and implicit Runge-Kutta methods are described for convenience. More details can be found in refs. [5, 6].

### 3.1 Discontinuous Galerkin method

The discontinuos Galerkin method of degree $q$ can be stated as: find $y$ (polynomial of degree $q$) such that

$$\int_{t_n}^{t_{n+1}} (\dot{y} + \lambda y) w \; dt + [y_n] \, w_n^+ = \int_{t_n}^{t_{n+1}} f w \; dt \tag{5}$$

For the weight functions $w$ polynomials of degree $q$ are used. The notations $y_n^+$ ja $y_n^-$ are the limits $y_n^\pm = \lim_{\epsilon \to 0} y(t_n \pm |\epsilon|)$, $[y_n] = y_n^+ - y_n^-$

Discontinuos Galerkin method allows the use of piecewise constant trial and weight functions. In this case $w = 1$ and the dG(0) method can be stated as follows

$$\int_{t_n}^{t_{n+1}} \lambda y \; dt + y_n^+ = y_n^- + \int_{t_n}^{t_{n+1}} f \; dt \tag{6}$$

Since $y$ is constant on the time step $(t_n, t_{n+1})$, therefore the following notations are used: $y_{n+1} = y_{n+1}^- = y_n^+$, resulting in the dG(0) method:

$$(1 + \gamma_{n+1}) y_{n+1} = y_n + \int_{t_n}^{t_{n+1}} f \; dt \tag{7}$$

where

$$\gamma_{n+1} = \int_{t_n}^{t_{n+1}} \lambda \; dt \tag{8}$$

For constant $\lambda$ and without the source term ($f = 0$), the dG(0) method is identical to the implicit Euler scheme.

### 3.2 Implicit Runge-Kutta methods

An $s$-stage implicit Runge-Kutta method for the solution of

$$\dot{y} = f(t, y) \tag{9}$$

can be defined as

$$k_i = y_0 + \Delta t \sum_{j=1}^{s} a_{ij} f(t_0 + c_j \Delta t, k_j) \quad i = 1, \ldots, s \tag{10}$$

$$y_1 = y_0 + \Delta t \sum_{j=1}^{s} b_j f(t_0 + c_j \Delta t, k_j) \tag{11}$$

The two stage Lobatto III C method is obtained when the coefficients have the values: $a_{11} = a_{21} = a_{22} = -a_{12} = 1/2, c_1 = 0, c_2 = 1, b_1 = b_2 = 1/2$.

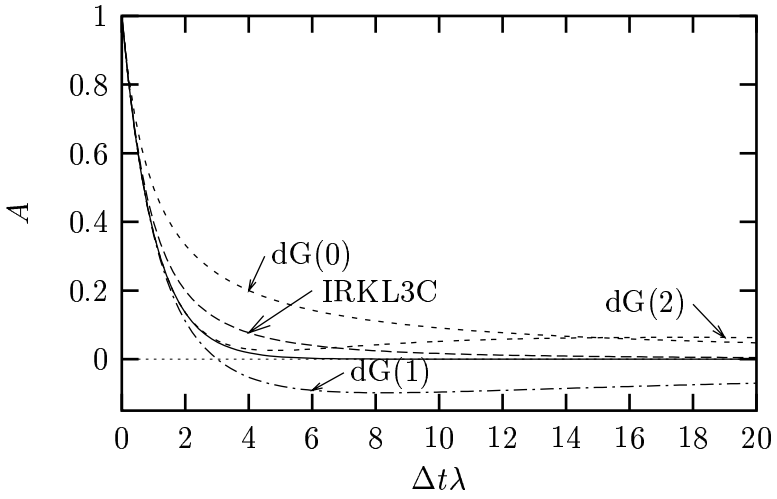


Figure 1: Amplification factors of different time integrators for the model problem $\dot{y} + \lambda y = 0$. Solid line represents the exact value.

### 3.3 Amplification factors

Amplification factors (or stability functions) reveal the basic properties of an integrator in question. Amplification factors of the asymptotically first, third and fifth order accurate discontinuos Galerkin time integrators and the two stage implicit Runge-Kutta Lobatto IIIC type integrator for the problem $\dot{y} + \lambda y = 0$ are

$$A_{\mathrm{bE}} = A_{\mathrm{dG}(0)} = \frac{1}{1 + \lambda\Delta t} \tag{12}$$

$$A_{\mathrm{dG}(1)} = \frac{1 - \frac{1}{3}\lambda\Delta t}{1 + \frac{2}{3}\lambda\Delta t + \frac{1}{6}(\lambda\Delta t)^2} \tag{13}$$

$$A_{\mathrm{dG}(2)} = \frac{1 - \frac{2}{5}\lambda\Delta t + \frac{1}{20}(\lambda\Delta t)^2}{1 + \frac{3}{5}\lambda\Delta t + \frac{3}{20}(\lambda\Delta t)^2 + \frac{1}{60}(\lambda\Delta t)^3} \tag{14}$$

$$A_{\mathrm{IRKL3C}} = \frac{1}{1 + \lambda\Delta t + \frac{1}{2}(\lambda\Delta t)^2} \tag{15}$$

and they are shown in fig. 1. It is clearly seen that the higher order Galerkin methods "looses" their accuracy as compared to the lowest order Galerkin method or the IRKL3C method when the time step is large.

As it is discussed in ref. [4], ideal time integrator for inelastic constitutive models should be $L$-stable and its amplification factor should be strictly positive and monotonous. The members of the dG(q) family when $q$ is odd, produce methods whose amplification factors tend to zero from the negative side. When $q$ is even, the amplification factors are strictly

positive but not monotonous. Therefore, except the dG(0)-method, none of the dG(q)-schemes has both these properties.

As it can be seen from fig. 1, the two stage Lobatto IIIC type IRK-method has the amplification factor which is equal to the Padé (0,2)-approximation of $\exp(-\lambda t)$, and thus exhibits the desired features. In general, the Padé $(0,q)$-approximations of $\exp(-\lambda t)$ are positive and monotonous.

## 4 A constrained discontinuos Petrov-Galerkin method

### 4.1 Autonomous constant coefficient case

It is now shown, that in the linear constant coefficient case the same approximation as produced by the IRKL3C-scheme, can also be obtained by modifying the dG(1) scheme. In this modified discontinuous Petrov-Galerkin type method the standard linear interpolation is used for the unknown function, but quadratic interpolation is used for the weight function $N_2^w$:

$$y = N_1 y_n^+ + N_2 y_{n+1}^- \quad \text{and} \quad w = N_1^w \omega_1 + N_2^w \omega_2 \tag{16}$$

where $N_1 = 1-\xi, N_2 = \xi$, $N_1^w = 1, N_2^w = \xi + \alpha\xi^2$ and $\xi = (t-t_n)/\Delta t$.[1] Substituting the interpolation and weight functions into (5) gives

$$\begin{pmatrix} \omega_1 \\ \omega_2 \end{pmatrix}^T \left[ \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} y_n^+ \\ y_{n+1}^- \end{pmatrix} + (y_n^+ - y_n^-) \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \right] = 0 \tag{17}$$

where

$$\begin{aligned} A_{ij} &= m_{ij} + k_{ij} \quad m_{ij} = \int_{t_n}^{t_{n+1}} N_i^w \dot{N}_j \, dt \\ k_{ij} &= \int_{t_n}^{t_{n+1}} \lambda N_i^w N_j \, dt \quad f_i = \int_{t_n}^{t_{n+1}} f N_i^w \, dt \end{aligned} \tag{18}$$

Solution of $y_{n+1}^-$ as a function of $y_n^-$ gives the amplification factor (assuming $f = 0$)

$$A = \frac{p_0 + p_1}{q_0 + q_1 + q_2} \tag{19}$$

where

$$\begin{aligned} p_0 &= -m_{21} & p_1 &= -k_{21} \\ q_0 &= (1+m_{11})m_{22} - m_{12}m_{21} & q_1 &= k_{11}m_{22} + k_{22}(1+m_{11}) - k_{12}m_{21} - k_{21}m_{12} \\ q_2 &= k_{11}k_{22} - k_{12}k_{21} \end{aligned} \tag{20}$$

Requiring the term $k_{21}$ to vanish, gives a value $\alpha = -2$ to the free parameter in the interpolation function $N_2^w$, if $\lambda$ is constant. Straightforward calculation shows the resulting amplification factor to be equal to the (0,2)-Padé approximation of $\exp(-\lambda t)$.

[1] This is only a convenient choice.

### 4.2 Generalisation

When the $\lambda$-coefficient is not constant, the constraint to the $\alpha$ will depend on it. Using linear interpolation for $\lambda$, i.e. $\lambda(t) = N_1\lambda_n + N_2\lambda_{n+1}$, gives the following constraint

$$\alpha = -\frac{5(\lambda_n + \lambda_{n+1})}{2\lambda_n + 3\lambda_{n+1}} \tag{21}$$

where $\lambda_n = \lambda(t_n), \lambda_{n+1} = \lambda(t_{n+1})$.

As it is shown in ref. [4] it is important to consider the behaviour of the integrator with the source term ($f$ in eq. 2). In this case solution for $y^-_{n+1}$ is given by equation

$$y^-_{n+1} = \frac{-A_{21}}{(1+A_{11})A_{22} - A_{12}A_{21}} y^-_n + \frac{(1+A_{11})f_2 - A_{21}f_1}{(1+A_{11})A_{22} - A_{12}A_{21}} \tag{22}$$

Requiring the term $k_{21}$ to vanish, it can be written

$$y^-_{n+1} = \frac{y^-_n + f_1 + (1+m_{11})(f_2/m_{22}) + k_{11}(f_2/m_{22})}{1 + k_{11} + k_{12} + (1+m_{11})(k_{22}/m_{22}) + k_{11}k_{22}/m_{22}} \tag{23}$$

Assuming now $y_{\mathrm{ref}} = y_0$, eq. (3) and $n = 0$, the amplification factor has the form

$$A = \frac{1 + \eta\lambda_0\Delta t(1 + \frac{1}{6}(2 + \lambda_1/\lambda_0)\lambda_0\Delta t)}{1 + \frac{1}{2}(\lambda_0 + \lambda_1)\Delta t + a(\lambda_0\Delta t)^2} \tag{24}$$

where

$$a = \frac{(2 + \lambda_1/\lambda_0)\,[1 + 6\lambda_1/\lambda_0 + 3(\lambda_1/\lambda_0)^2]}{12(4 + \lambda_1/\lambda_0)} \tag{25}$$

Notice, that $a \to \frac{1}{2}$ when $\lambda_1 \to \lambda_0$.

For comparison, the Lobatto IIIC type IRK-method has the amplification factor

$$A_{\mathrm{IRKL3C}} = \frac{1 + \eta\lambda_0\Delta t(1 + \frac{1}{2}\lambda_0\Delta t)}{1 + \frac{1}{2}(\lambda_0 + \lambda_1)\Delta t + \frac{1}{2}\lambda_0\lambda_1(\Delta t)^2} \tag{26}$$

In numerical tests the dPG(1)-method, when integrating all terms exactly, seems not to be as accurate as the IRKL3C-method. However, when two-point Gauss-Lobatto quadrature is used for the dPG(1)-method, it will yield exactly the IRKL3C-method (26). The coefficients have now the values:

$$m_{11} = -1 \qquad m_{12} = 1 \qquad m_{21} = -\tfrac{1}{2}(1+\alpha) \qquad m_{22} = \tfrac{1}{2}(1+\alpha) \tag{27}$$

$$k_{11} = \tfrac{1}{2}\lambda_0\Delta t \qquad k_{12} = \tfrac{1}{2}\lambda_1\Delta t \qquad k_{21} = 0 \qquad k_{22} = \tfrac{1}{2}\lambda_1(1+\alpha)\Delta t \tag{28}$$

In this case, the value for the $\alpha$-parameter is irrelevant, since $k_{22}/m_{22} = \frac{1}{2}\lambda_1\Delta t$, see eq. (22).

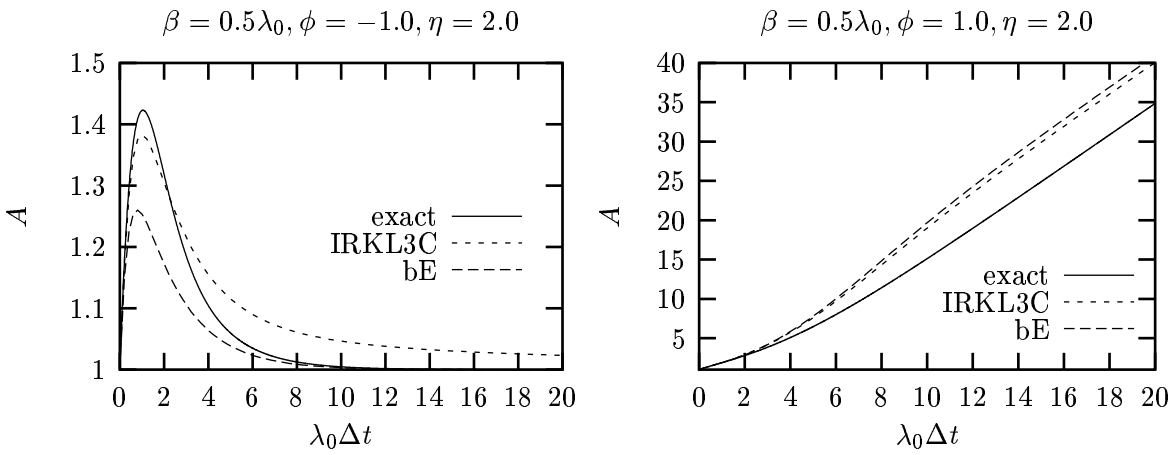


Figure 2: Amplification factors.

It can also be noticed, that the dG(1)-method will be equivalent to the two-stage implicit Runge-Kutta Lobatto III C type method when the integrals are evaluated by the two-point Gauss-Lobatto quadrature. The coefficients have now the values:

$$m_{11} = -\tfrac{1}{2} \qquad m_{12} = \tfrac{1}{2} \qquad m_{21} = -\tfrac{1}{2} \qquad m_{22} = \tfrac{1}{2} \tag{29}$$

$$k_{11} = \tfrac{1}{2}\lambda_0 \Delta t \qquad k_{12} = 0 \qquad k_{21} = 0 \qquad k_{22} = \tfrac{1}{2}\lambda_1 \Delta t \tag{30}$$

Therefore asymptotically third order accurate scheme can be obtained by changing the two-point Gauss-Lobatto integration to two-point Gauss-Legendre integration, if the time step is sufficiently small and the estimation of it is available. The dG(1)-scheme should not be used for large time steps. However, the Lobatto underintegrated scheme is robust and second order accurate also in the asymptotic range.

Comparison between the backward Euler and the two-stage IRKL3C-method is shown in fig. 2 for the non-autonomous model problem (2) where the diffusion coefficient $\lambda$ is defined as

$$\lambda(t) = \lambda_0 \left[1 - \phi + \phi \exp(-\beta t)\right] \tag{31}$$

For large time steps the backward Euler method is more accurate than the IRKL3C-scheme for the increasing diffusivity case ($\phi = -1$), shown on the lhs in fig. 2. On the rather extreme case of vanishing diffusivity ($\phi = 1$, then $\lambda \to 0$ when $t \to \infty$) both integrators behave similarly.

# 5 NUMERICAL EXPERIMENTS

## 5.1 Material model

A creep type inelastic material model is used in the following example. In this model, the inelastic strain is assumed to be strictly deviatoric and the evolution equation for the inelastic strain rate can be written as

$$\dot{\boldsymbol{\epsilon}}^{\text{in}} = \tfrac{3}{2}\gamma\mathbf{n}, \qquad \text{where} \qquad \mathbf{n} = (\mathbf{s} - \tfrac{2}{3}\mathbf{B})/\bar{\tau} \tag{32}$$

The scalar $\bar{\tau}$ is the reduced equivalent stress

$$\bar{\tau} = \sqrt{\tfrac{3}{2}\boldsymbol{\tau}{:}\boldsymbol{\tau}} = \sqrt{\tfrac{3}{2}\left(\mathbf{s} - \tfrac{2}{3}\mathbf{B}\right) : \left(\mathbf{s} - \tfrac{2}{3}\mathbf{B}\right)} \tag{33}$$

where $\mathbf{s}$ is the stress deviator and $\mathbf{B}$ is the back stress accounting for the kinematic hardening. A widely used stress function to model secondary creep is due to Garofalo [7]

$$\gamma = f^* \exp\left(\frac{-Q}{R\theta}\right) \sinh^m\left(\frac{\bar{\tau}}{\sigma_y}\right) \tag{34}$$

where $Q$ is the process activation energy, $R$ is the gas constant and $\theta$ the absolute temperature. In this study, the exponent $m$ and the coefficient $f$ are assumed to be constant, although they depend on the grain size [7].

Hardening rules are adopted from the constitutive model of Miller [8], which are also used in refs. [9, 10, 11, 12]:

$$\begin{aligned} \dot{\sigma}_y &= H_1\gamma - (H_2\gamma + H_3)(\sigma_y - \sigma_{y,0})^2 \\ \dot{\mathbf{B}} &= K_1\dot{\boldsymbol{\epsilon}}^{\text{in}} - (K_2\gamma + K_3)\bar{B}\mathbf{B} \end{aligned} \tag{35}$$

where $H_1, ...., H_3, K_1, ..., K_3$ and $Y_0$ are material parameters and $\bar{B} = \sqrt{\frac{2}{3}\mathbf{B} : \mathbf{B}}$.

## 5.2 Bar in uniaxial tension

A bar strained uniaxially with a constant strain rate $10^{-5}$ is analysed using a single tri-linear brick element. Behaviour of the bE, dG(0) and the two stage IRKL3C type method (equivalent to the dG(1) method with two point Lobatto integration) is studied. Computed stress-strain relations are shown in fig. 3. Thermally softening and hardening cases have been studied. Temperature is assumed to change linearly with time $\theta(t) = \theta_0 \pm \Delta\theta(t/t_{\max})$, where $t_{\max} = \epsilon_{\max}/\dot{\epsilon}$ and $\theta_0 = 293$ K, $\Delta\theta = 40$ K. Increase or decrease in temperature result in softening or hardening behaviour, respectively. The material parameters used corresponds to the binary near eutectic Sn40Pb solder and are the following [10]: $E = 33$ GPa, $Q = 12$ kcal/mol, $\nu = 0.3$, $R = 2{\cdot}10^{-3}$ kcal/mol·K, $\sigma_y = 20$ MPa, $f = 10^5$ s$^{-1}$, $m = 3.5$.

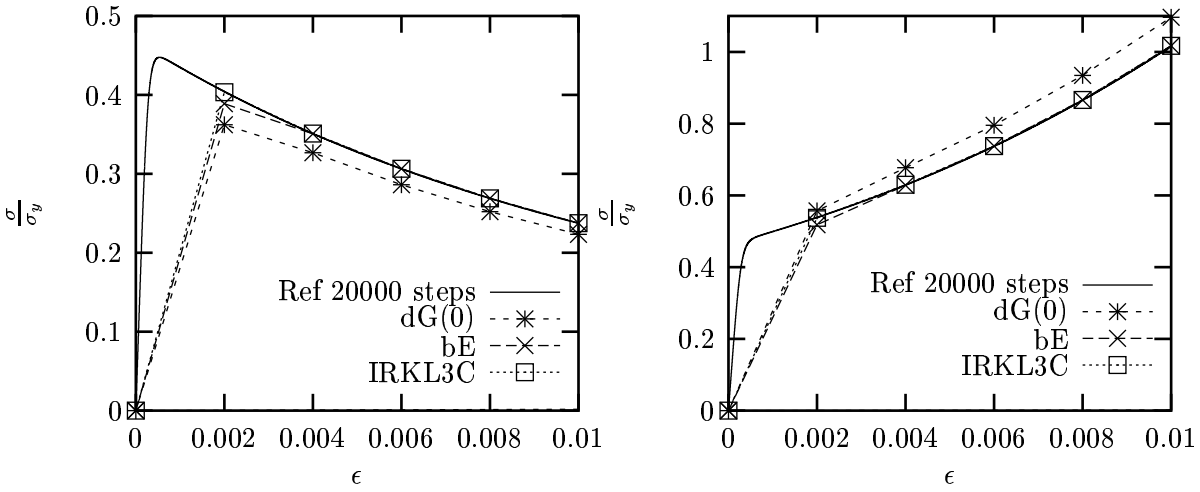


Figure 3: Uniaxial straining, strain rate $10^{-5}$.

For the thermally hardening case, the relative error at the end of computation ($t = t_{\max}$) is shown as a function of time step in fig. 4 when using the strain rate $\dot{\epsilon} = 10^{-5}$. Both the backward Euler and the discontinuous Galerkin method with piecewise constant trial functions are asymptotically first order accurate. However, the error constant for the backward Euler scheme is significantly smaller than for the dG(0)-method, as shown in ref. [4]. The two stage IRKL3C method, which is equal to the dG(1)-method with two point Gauss-Lobatto integration is clearly the most accurate also for large time steps.

## 6 CONCLUSIONS

The backward Euler scheme is a popular time-integrator for inelastic constitutive models. Although it is asymptotically only first order accurate, it yields accurate solutions when the time step is large, which is relevant to practical computations. The asymptotically second order two-stage Lobatto IIIC type implicit Runge-Kutta method has good accuracy also for large time steps. It is also shown that the two-stage Lobatto IIIC scheme can be formulated with the discontinuous Galerkin approach by either using specific weight-functions or using Gauss-Lobatto quadrature to underintegrate the coefficients in the dG(1)-method.

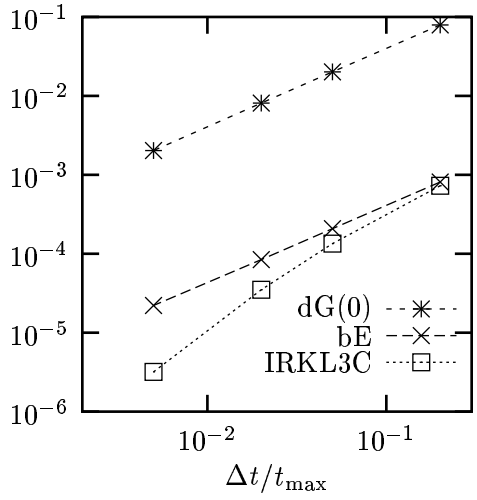


Figure 4: Uniaxial straining, relative error as a function of time step, constant strain rate $10^{-5}$.

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