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DETERMINATION OF TIME STEP IN AN IMPLICIT DIFFERENCE SCHEME FOR SOLVING THE NONLINEAR HEAT CONDUCTION EQUATION ON AN UNSTRUCTURED 3D MESH

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RFNC-VNIITF named after Academ. E.I.Zababakhin, Snezhinsk

Convergence condition

Nonlinear heat conduction equation

$$\rho \frac{\partial \varepsilon}{\partial t} - \nabla \cdot \left(\kappa(\rho, T) \nabla T \right) = \rho Q$$

$\varepsilon(\rho, T)$ - internal energy, $\rho\left(\vec{r}\right)$ - density.

Implicit semi-discrete scheme

$$\rho \frac{\varepsilon^{n+1} - \varepsilon^{n}}{\Delta t} - \nabla \cdot \left(\kappa(T^{n+1}) \nabla T^{n+1} \right) = \rho Q^{n+1/2} \qquad (1)$$

Iterative process is used for solution

$$\rho \frac{\varepsilon^{\nu} + \left(\frac{\partial \varepsilon}{\partial T} \right)^{\nu} \left(T^{\nu+1} - T^{\nu} \right) - \varepsilon^{n}}{\Delta t} - \nabla \cdot \left(\kappa(T^{\nu}) \nabla T^{\nu+1} \right) = \rho Q^{n+1/2} \qquad (2)$$

Solution on each iteration is deviation of solution from n+1 layer $T^{\nu} = T^{n+1} + \delta T^{\nu}$, $T^{\nu+1} = T^{n+1} + \delta T^{\nu+1}$

$$\rho \frac{\varepsilon^{n+1} + \left(\frac{\partial \varepsilon}{\partial T} \right)^{n+1} \delta T^{\nu+1} - \varepsilon^{n}}{\Delta t} - \nabla \cdot \left[\kappa^{n+1} \nabla T^{n+1} + \kappa^{n+1} \nabla T^{\nu+1} + \left(\frac{\partial \kappa}{\partial T} \right)^{n+1} \nabla T^{n+1} \delta T^{\nu} \right] = \rho Q^{n+1/2} \qquad (3)$$

To subtract (1) from (3)

$$\rho \frac{\left(\frac{\partial \varepsilon}{\partial T} \right)^{n+1} \delta T^{\nu+1}}{\Delta t} - \nabla \cdot \left[\kappa^{n+1} \nabla T^{\nu+1} + \left(\frac{\partial \kappa}{\partial T} \right)^{n+1} \nabla T^{n+1} \delta T^{\nu} \right] = 0 \qquad (4)$$

Y.A. Bondarenko, A.A. Gorbunov, Practical stability condition for heat wave calculation with implicit difference scheme. Journal VANT, MMFP Series, - 2008. - V.4.- P.3-12.

Convergence condition

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Consider one dimensioned case and introduce space discretization on uniform mesh

Assumption: κ and $\left(\partial\kappa/\partial T\right)\nabla T$ are not depend on grid pattern

$$\delta T_i^{\nu+1} - K_0^{n+1}\left(\delta T_{i+1}^{\nu+1} - 2\delta T_i^{\nu+1} + \delta T_{i-1}^{\nu+1}\right) + \frac{\sigma}{2} K_{\alpha\beta}^{n+1}\left(\delta T_{i+1}^{\nu} - \delta T_{i-1}^{\nu}\right) = 0$$

$$K_0^{n+1} = \frac{\Delta t \kappa_i^{n+1}}{\Delta x^2 \rho_i \left(\frac{\partial \varepsilon}{\partial T}\right)_i^{n+1}}$$

Courant number for heat conductivity in case of explicit scheme

$$K_{TV}^{n+1} = \frac{\Delta t \left|q_i^{n+1}\right|}{\Delta x \rho_i \varepsilon_i^{n+1}}$$

Courant number of heat transfer

$$q_i^{n+1} = -\kappa_i^{n+1} \nabla T_i^{n+1}$$

Heat flow

$$K_{\alpha\beta}^{n+1} = K_{TV}^{n+1} \frac{\alpha^{n+1}}{\beta^{n+1}}$$

$$\alpha^{n+1} = \frac{T_i^{n+1}}{\kappa_i^{n+1}}\left(\frac{\partial \kappa}{\partial T}\right)_i^{n+1}, \quad \beta^{n+1} = \frac{T_i^{n+1}}{\varepsilon_i^{n+1}}\left(\frac{\partial \varepsilon}{\partial T}\right)_i^{n+1}$$

Factor of nonlinear dependence of heat conductivity factor and internal energy

Convergence condition

Find stability condition of scheme for δT by Neumann method (convergence condition of iterative process):

$$\delta T_j^{\nu} = \delta T_0 \gamma^{\nu} e^{ij\omega}$$

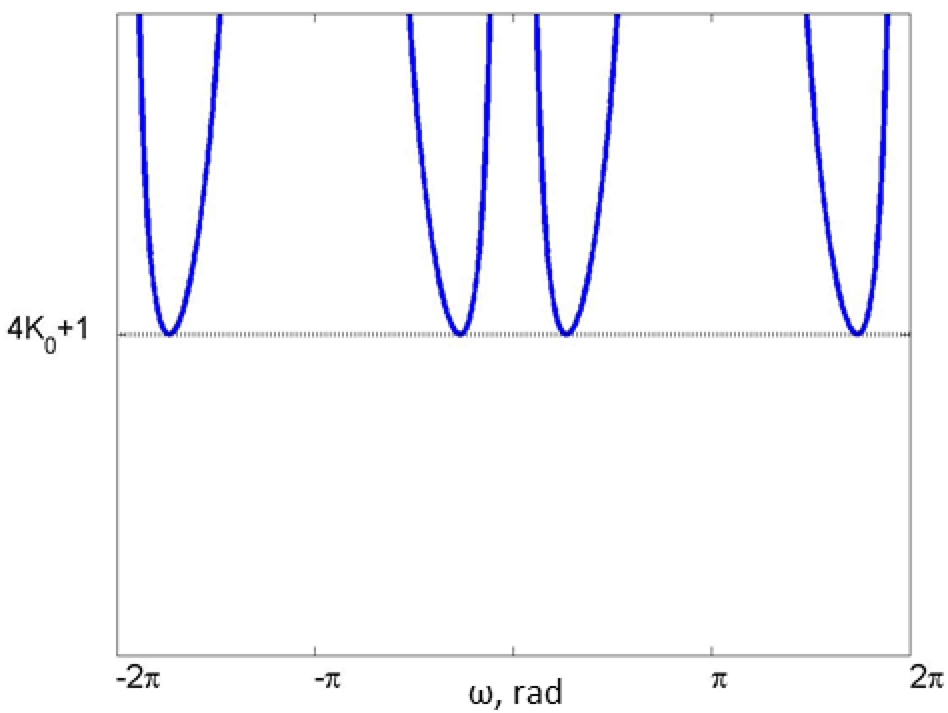
$$|\gamma| = \left| \frac{-\sigma i K_{\alpha\beta}^{n+1} \sin\omega}{1 + 2K_0^{n+1}(1-\cos\omega)} \right| < 1$$

$$\Updownarrow$$

$$\left(K_{\alpha\beta}^{n+1}\right)^2 < \frac{\left(1 + 2K_0^{n+1}(1-\cos\omega)\right)^2}{\sin^2\omega}$$

$$\Uparrow$$

$$\left(K_{\alpha\beta}^{n+1}\right)^2 < 4K_0^{n+1} + 1$$



Practical condition of time step

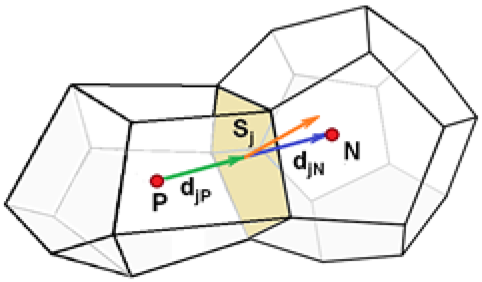
$$\Delta t^{n+1} < \frac{4\dfrac{\kappa_i^n}{\rho_i \left(\partial\varepsilon/\partial T\right)_i^n}}{\left(\dfrac{q^n}{\rho_i \varepsilon_i^n} \dfrac{\alpha_i^n}{\beta_i^n}\right)^2} = \frac{4\Delta t^n \left(K_0\right)_i^n}{\left(\left(K_{TV}\right)_i^n \dfrac{\varepsilon_i^n}{T_i^n} \dfrac{\alpha_i^n}{\left(\partial\varepsilon/\partial T\right)_i^n}\right)^2}$$

Numerical scheme of nonlinear heat conduction equation in Focus*

Space discretization – finite volume method

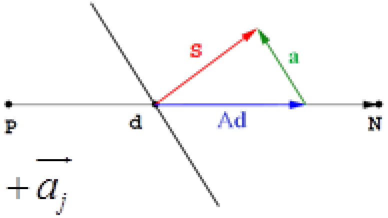
$$\rho_i \frac{\partial \varepsilon_i}{\partial t} - \frac{1}{|V_i|}\int_{V_i} \nabla\cdot(\kappa(\rho,T)\nabla T)dV = \rho_i Q_i, \quad \varepsilon_i \equiv \int_{V_i} \varepsilon\, dV/|V_i|, \quad Q_i \equiv \int_{V_i} Q\, dV/|V_i|,$$

$$\frac{\varepsilon_i^{n+1}-\varepsilon_i^n}{\Delta t} - \frac{1}{M_i}\sum_j \kappa_j(\rho,T^{n+1})\nabla T_j^{n+1}\overrightarrow{S_j} = Q_i^{n+1/2},$$



Iterative algorithm

$$\frac{\varepsilon_i^{\nu} + \left(\frac{\partial \varepsilon}{\partial T}\right)_i^{\nu}\left(T_i^{\nu+1}-T_i^{\nu}\right) - \varepsilon_i^n}{\Delta t} - \frac{1}{M_i}\sum_j \kappa_j(\rho,T^{\nu})\nabla T_j^{\nu+1}\overrightarrow{S_j} = Q_i^{n+1/2}$$



Normal temperature gradient to face

$$\nabla T_j^{\nu+1}\overrightarrow{S_j} \approx A_j\left(T_N^{\nu+1}-T_P^{\nu+1}\right) + \overrightarrow{a_j}\cdot(\nabla T)_j^{\nu}, \quad A_j = \frac{\left|\overrightarrow{S_j}\right|^2}{\overrightarrow{d_j}\,\overrightarrow{S_j}}, \quad \overrightarrow{S_j} = A_j\overrightarrow{d_j} + \overrightarrow{a_j}$$

Heat conductivity factor on faces

$$\frac{1}{2\kappa_j^{sh}} = \frac{1-\omega_j}{\kappa_P + \kappa_j^{lin}} + \frac{\omega_j}{\kappa_N + \kappa_j^{lin}}, \qquad \kappa_j^{sh} = \frac{\left(\kappa_P + \kappa_j^{lin}\right)\left(\kappa_N + \kappa_j^{lin}\right)}{4\kappa_j^{lin}}.$$

* N.A. Mikhaylov, I.V. Glazyrin, Method of contact bound steepening for the simulation of 3D multiphase compressible flows in Euler variables. ZST: collection of thesis XIII international conference 20-24 March 2017. – Snezhinsk: FSUE "RFNC-VNIITF named after Academ. E.I.Zababakhin" – P.326.

Time step limit in Focus

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$$\Delta t^{n+1} = \min_{i:K_0>K_{\min}} \left[\frac{4\Delta t^n (K_0)_i^n}{\left((K_{TV})_i^n \frac{\varepsilon_i^n}{T_i^n} \frac{\alpha_i^n}{(\partial\varepsilon/\partial T)_i^n} \right)^2} \right] \qquad K_{\min} = 1.0$$

$$K_0^n \equiv \frac{\Delta t \kappa_i^n}{\Delta x^2 \rho (\partial\varepsilon/\partial T)_i^n} \approx \left[\frac{\kappa_i^n}{\Delta x^2} \approx \frac{\sum_j \kappa_j S_j / d_j}{V_i} \right] \approx \frac{\Delta t}{(\partial\varepsilon/\partial T)_i^n} \frac{\sum_j (\kappa_j A_j)}{\rho_i V_i N_{face}}, \quad A_j = \frac{\left|\vec{S_j}\right|^2}{\vec{d_j}\vec{S_j}}$$

- Courant number for heat conductivity in case of explicit scheme

$$K_{TV}^n \equiv \frac{\Delta t \left|q_i^n\right|}{\Delta x \rho \varepsilon_i^n} \approx \frac{\Delta t}{\varepsilon_i^n \rho_i V_i} \max_j \left|q_{ij}^n\right|$$

- Courant number of heat transfer

$$\left|q_{ij}^n\right| = \kappa_j \nabla T_j^n \cdot \vec{S_j}$$

- Heat flow

$$\kappa_i = \frac{\sum_j \kappa_j \vec{S_j}}{\sum_j \vec{S_j}}, \quad \left(\frac{\partial\kappa}{\partial T}\right)_i = \frac{\sum_j \left(\frac{\partial\kappa}{\partial T}\right)_j \vec{S_j}}{\sum_j \vec{S_j}}$$

- Average values on faces

Difference from MEDUZA*

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$$K_0^n = \frac{\Delta t \kappa_i^n}{\Delta x^2 \left(\partial\varepsilon/\partial T\right)_i^n} = \frac{\Delta t}{\left(\partial\varepsilon/\partial T\right)_i^n} \frac{1}{N_{side}} \sum_k \max_l \left|\alpha_{kl}^n\right|$$

- Courant number for heat conductivity in case of explicit scheme

$$K_{TV}^n = \frac{\Delta t \left|q_i^n\right|}{\Delta x \varepsilon_i^n} = \frac{\Delta t \max\limits_k \left|q_{ik}^n\right|}{\max\left(\varepsilon_i^n, \theta^2 \max\limits_k \varepsilon_k^n\right)}, \quad \theta = 10^{-2}$$

- Courant number of heat transfer

Factor of nonlinear dependence of heat conductivity factor

$$\alpha_i = \frac{T_i}{\kappa_i}\left(\frac{\partial\kappa}{\partial T}\right)_i \approx \frac{\partial \ln\kappa/\partial x}{\partial \ln T/\partial x} \approx \frac{\ln\kappa_i\left(T_i^n\right) - \ln\kappa_i\left(T_j^n\right)}{\ln T_i^n - \ln T_j^n} \approx \max\left\{\alpha_{\min}, \max_k \frac{\ln\dfrac{\kappa_i\left(T_i^n\right)}{\kappa_i\left(T_{ik}^n\right)}}{\ln\dfrac{T_i^n}{T_{ik}^n}}\right\}, \quad \alpha_{\min} = 1.0$$

*Y.A. Bondarenko, A.A. Gorbunov, Practical stability condition for heat wave calculation with implicit difference scheme. Journal VANT, MMFP Series, - 2008. - V.4. - P.3-12.

Test 1. Problem of progressive heat wave

Calculated area: $[0,1]\times[0,0.1]\times[0,0.1]$

Initial conditions : $T=1\cdot 10^{-10}$

Time: $t\in(0,0.2]$

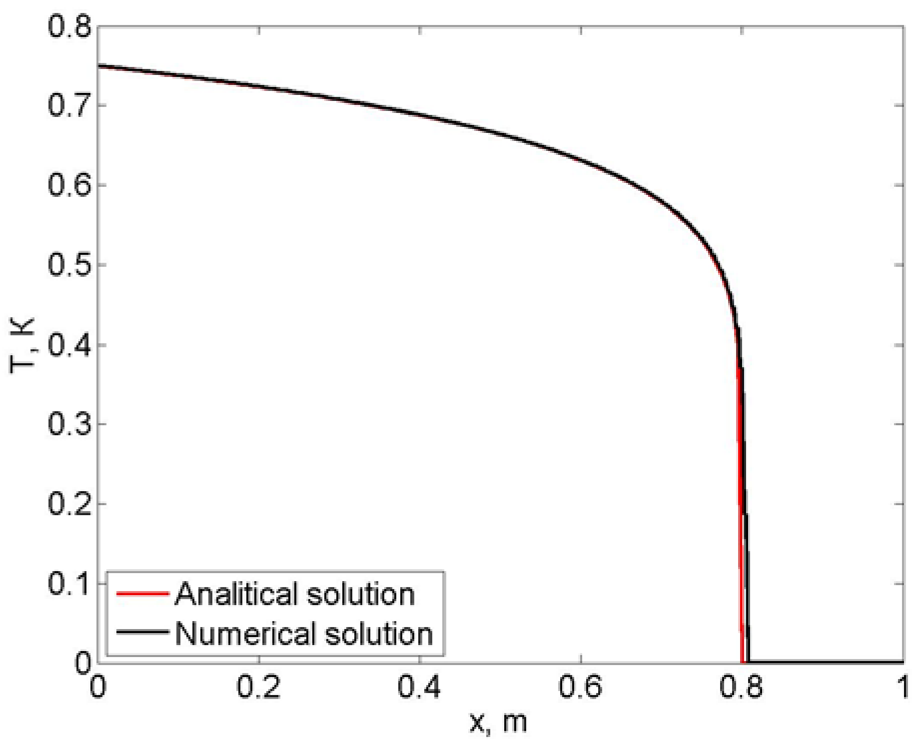
Boundary conditions :

1. Left bound: $T_{x=0}(t)=(0.5t)^{1/8}$
2. On the other bound: zero heat flux

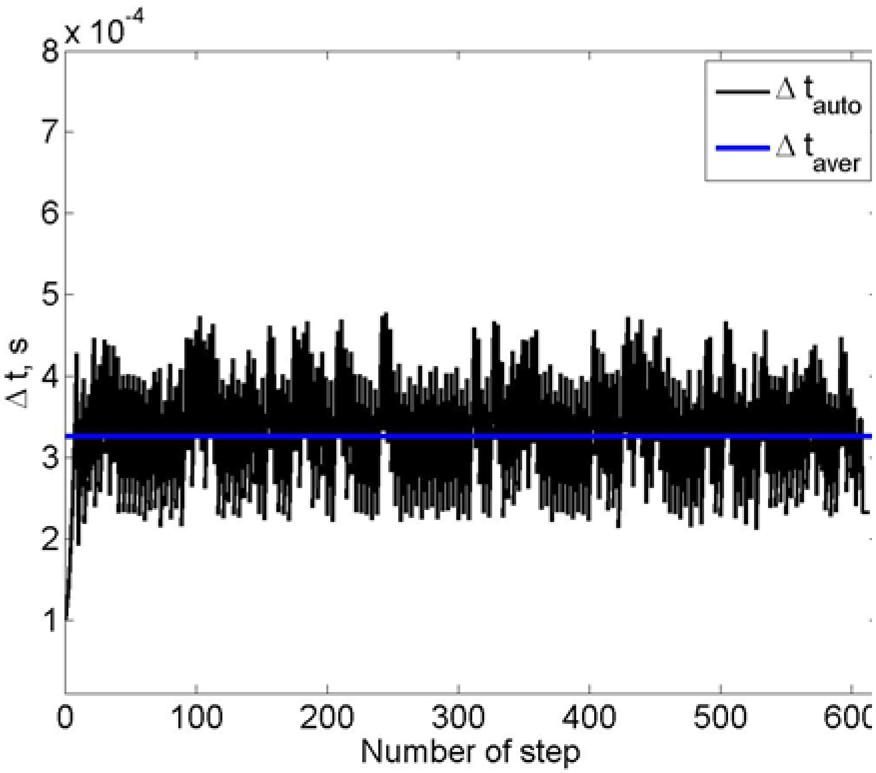
State equation and properties:

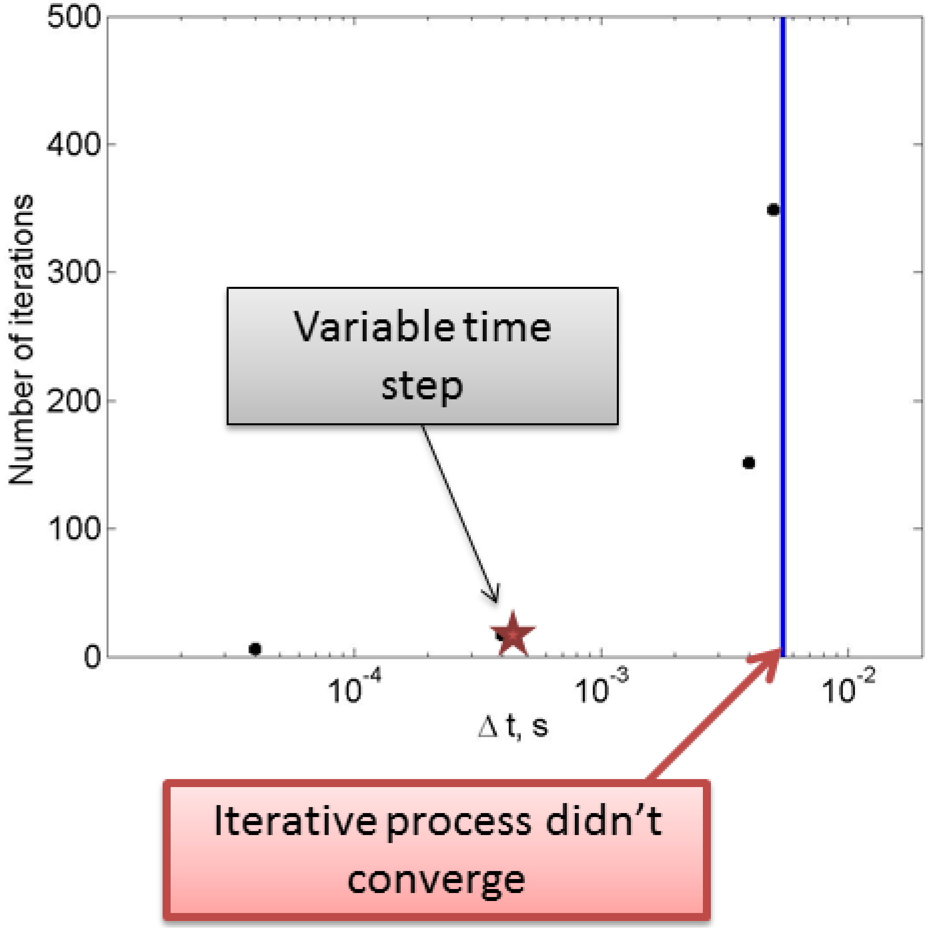
$$\varepsilon(T)=T,\quad \kappa=256T^{8},\quad \rho=1.$$

Grid: $[200\times20\times20]$



Number of iterations vs time step





Test 2. Problem of spherical heat wave

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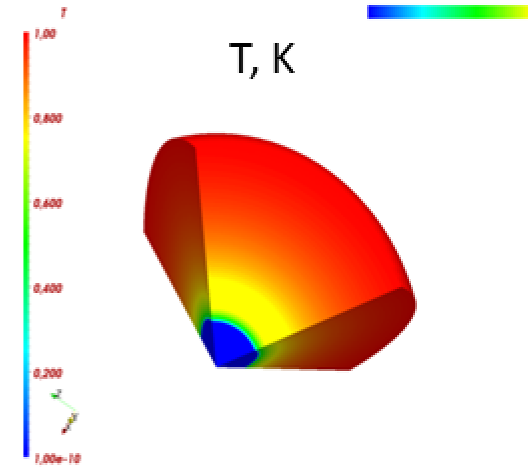
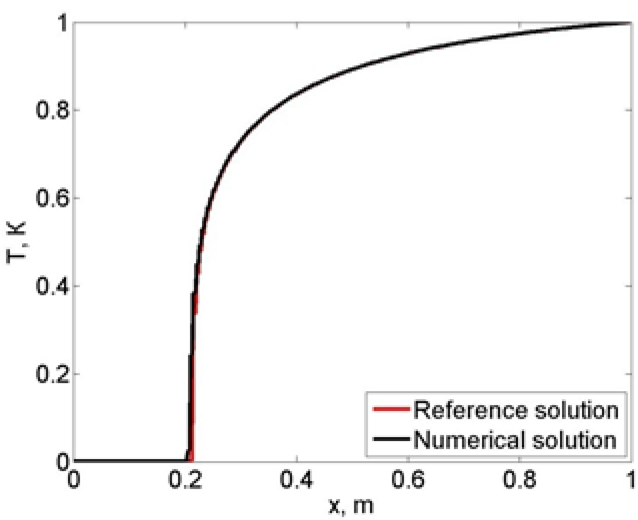
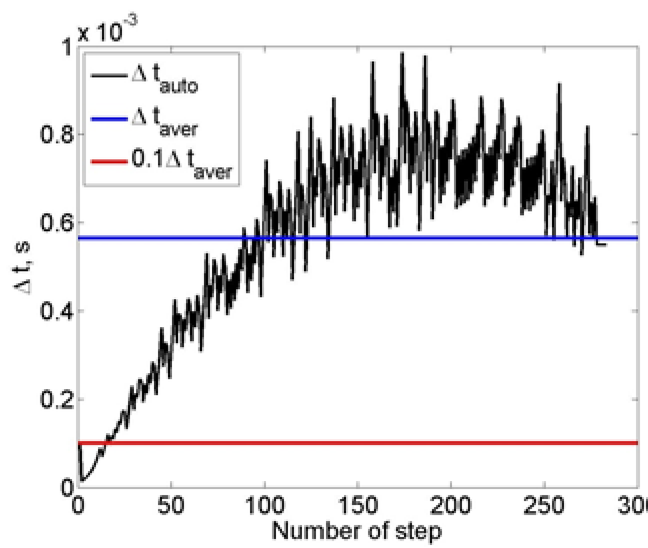
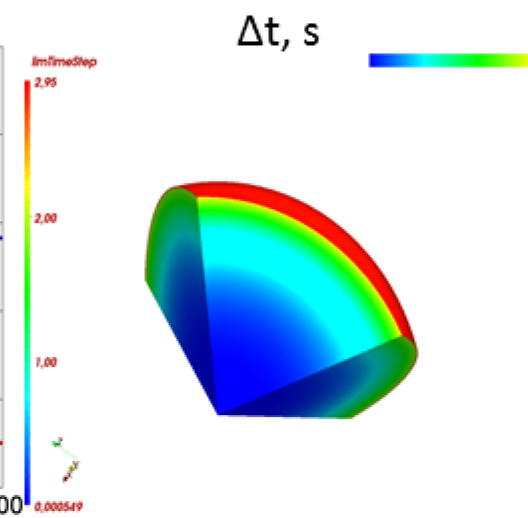
Calculated area: 1/6 part of sphere, radius of sphere $R=1$
Time: $t \in (0, 0.16]$
Initial conditions: $T = 1 \cdot 10^{-10}$
Boundary conditions: on outer surface of sphere $T_{R=1} = 1$
State equation and properties: $E = T,\ \ \rho = 1,\ \ \kappa = 4T^4$
Grid:
Radial: 18494, 155711, 1190892 cells.









Test 2. Problem of spherical heat wave

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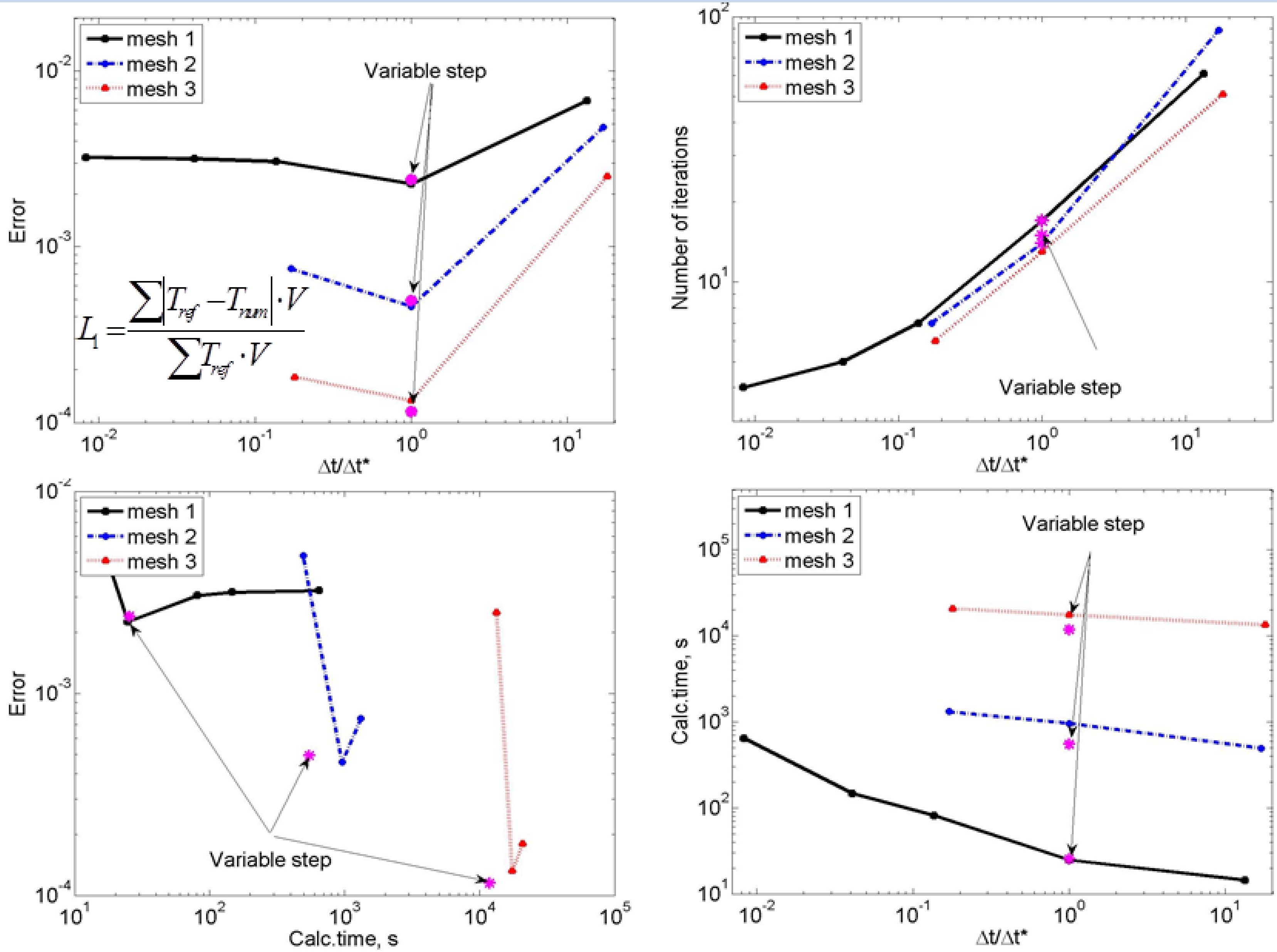

$$L_1 = \frac{\sum |T_{ref} - T_{num}| \cdot V}{\sum T_{ref} \cdot V}$$

Conclusion

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1. Iterative process may not converge without limiting time step Δt.
2. Time step condition Δt must take into account specifics of used numerical scheme.
3. Calculations of spherical heat wave test problem showed that the proposed time step limit Δt^* for Focus is more efficient as compared with fixed time step.
4. If accounting complementary processes, for example, hydrodynamics, it is necessary to introduce additional limit on number of iterations, since the calculating time of heat conductivity can exceed calculating time of other processes.

Thank you for attention!