Explicit, stable numerical methods
for
diffusion-reaction equations
and
heat transfer problems

Dr. Endre Kovács

University of Miskolc,
Department of Physics and Electric Engineering

Members of the research group

PhD students:

Mahmoud Saleh

Issa Omle

Ádám Nagy

Humam Kareem

Ali Habeeb Askar

Husniddin Khayrullaev

Dániel Koics

Other collaborators:

János Majár

Imre Barna

…

Equation for heat conduction or diffusion:

- Special case, 1D, homogeneous media

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} + q$$

- Where $u:[x_0, x_0 + L]\times[t_0, t_0 + T] \to \mathbb{R}$ is the concentration or temperature.

- General case, diffusivity has spatial dependence:

$$\alpha = \alpha(\vec{r}) = \frac{k(\vec{r})}{c(\vec{r})\rho(\vec{r})}$$

Then:

$$c\rho\frac{\partial u}{\partial t} = \nabla(k\nabla u) + c\rho q$$

Diffusion-reaction equations

- Linear reaction: $$\frac{\partial u}{\partial t} = \alpha \nabla^2 u - \beta u \qquad \beta \geq 0$$
- Fisher: $$\frac{\partial u}{\partial t} = \alpha \nabla^2 u + \beta u \left(1 - u\right)$$
- Huxley: $$\frac{\partial u}{\partial t} = \alpha \nabla^2 u + \beta u^2 \left(1 - u\right)$$
- Nagumo: $$\frac{\partial u}{\partial t} = \alpha \nabla^2 u + \beta u \left(1 - u^\delta\right)\left(u^\delta - \gamma\right)$$

Heat transfer equation

$$\frac{\partial u}{\partial t} = \frac{1}{c\rho}\nabla\left(k\nabla u\right) - K \cdot u - \sigma \cdot u^4 + q \qquad K, \sigma \geq 0$$

Convection
(Newton's law of cooling)

Radiation

(Stefan-Boltzmann Law)

Heat source
depends on ambient T and sunshine

Numerical methods

- Explicit methods: easy to code, parallelize
  one time step runs fast,
  Conditionally stable

- Implicit methods : a system of algebraic equations must be solved
  harder to code (unless built-in functions are used),
  hard to parallelize
  one time step is slower,
  Unconditional stability is frequent

Space Discretisation

- Central difference scheme: $$\frac{du_i}{dt} = \alpha \frac{u_{i-1} - 2u_i + u_{i+1}}{\Delta x^2} + q_i$$
- In a matrix form: $$\frac{d\vec{u}}{dt} = M\vec{u} + \vec{q} \qquad m_{ii} = -\frac{2\alpha}{\Delta x^2}, \quad m_{i,i+1} = m_{i,i-1} = \frac{\alpha}{\Delta x^2} \quad (1 < i < N)$$
- Stiffness ratio from the eigenvalues of M: $$SR = \lambda_{\max} / \lambda_{\min}$$
- CFL limit: $$h_{\mathrm{MAX}}^{\mathrm{EE}} = -2 / \lambda_{\max}$$

Discretisation of the time variable

- Uniform discretization: $t^n = nh\,, n \in \{0,1,2,\ldots,T\}$
- Mesh ratio: $r = \dfrac{\alpha h}{\Delta x^2} = -\dfrac{m_{ii}}{2}h\,, 1 < i < N$
- The ODE system, considered **inside one time step**:

$$\frac{du_i}{dt} = \alpha \frac{u_{i-1} - 2u_i + u_{i+1}}{\Delta x^2} + q_i \quad \Rightarrow \quad \frac{du_i}{dt} = -2\frac{r}{h}u_i + \underbrace{\frac{r}{h}u_{i\pm1} + q_i}_{(*)}$$

- Simplification will be made about the ***time*** of the (*) term.

The constant-neighbour (CNe) method

- The ODE system: $$\frac{du_i(t)}{dt} = -2\frac{r}{h}u_i(t) + \underbrace{\frac{r}{h}u_{i\pm1}(t) + q_i}_{a_i}$$

a_i ← constant in a timestep

We obtain $$\frac{du_i(t)}{dt} = a_i - 2\frac{r}{h}u_i(t)$$

$$a_i^n = \frac{r}{h}u_{i\pm1}^n + q_i^n$$

The simple analitical solution:

$$u_i(t) = u_i^0 \cdot e^{-2rt/h} + \frac{a_i h}{2r}\left(1 - e^{-2rt/h}\right)$$

The CNe formula:

$$u_i^{n+1} = u_i^n \cdot e^{-2r} + \frac{ha_i}{2r}\left(1 - e^{-2r}\right) = u_i^n \cdot e^{-2r} + \left(\frac{u_{i\pm1}^n}{2} + \frac{h}{2r}q_i\right)\left(1 - e^{-2r}\right)$$

The order of accuracy is **1**.

The CpC method

- The structure is similar to the explicit midpoint-method: two stages, both with the CNe formula

- 1. Predictor with halfed time step size

$$u_i^{\text{pred}} = u_i^n \cdot e^{-r} + \left(\frac{u_{i\pm1}^n}{2} + \frac{h}{2r} q_i \right) \left(1 - e^{-r}\right)$$

- 2. Corrector with full time step size

$$u_i^{n+1} = u_i^n \cdot e^{-2r} + \left(\frac{u_{i\pm1}^{\text{pred}}}{2} + \frac{h}{2r} q_i \right) \left(1 - e^{-2r}\right)$$

- Order of accuracy: **2**

The linear-neighbour (LNe) method

- The ODE system: $\dfrac{du_i(t)}{dt} = -2\dfrac{r}{h}u_i(t) + \underbrace{\dfrac{r}{h}u_{i\pm1}(t) + q_i}_{s_i t + a_i}$

where $s_i = \dfrac{a_i^{\text{pred}} - a_i}{h}$ is the slope, and $a_i^{\text{pred}} = \dfrac{r}{h}u_{i\pm1}^{\text{pred}} + q_i^{n+1}$

We need a predictor stage: CNe formula with full time step size.

The de-coupled ODE system: $\dfrac{du_i(t)}{dt} = s_i t + a_i - 2\dfrac{r}{h}u_i(t)$

It also has an analitical solution, based on which we get the LNe formula:

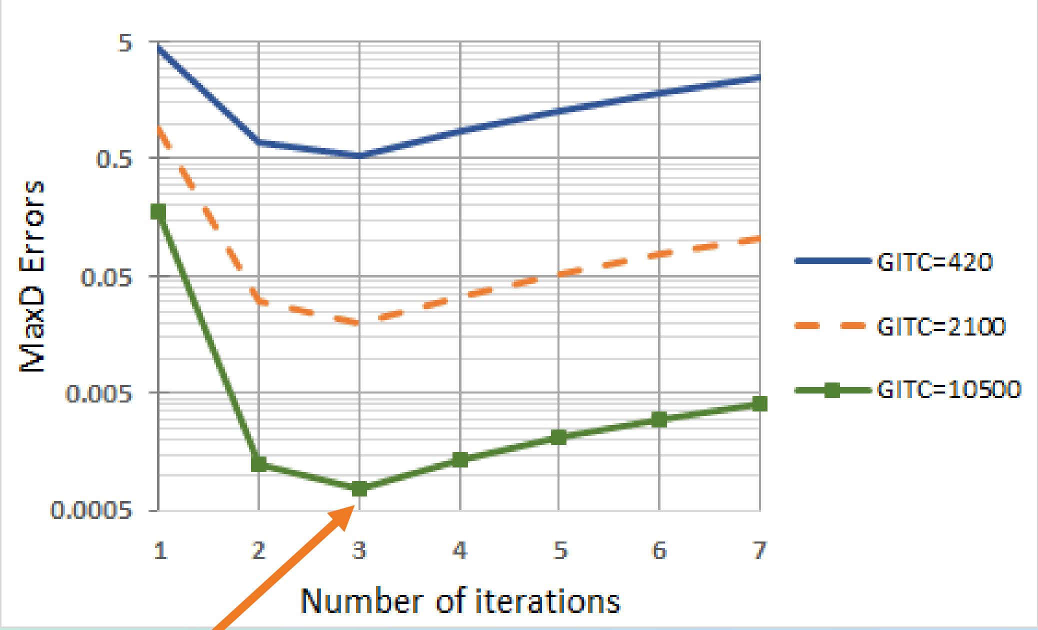
$$u_i^{\text{L},n+1} = u_i^n e^{-2r} + \frac{h}{2r}\left(\frac{1}{2r}\left(a_i - a_i^{\text{pred}}\right) + a_i\right)\left(1 - e^{-2r}\right) - \frac{h}{2r}\left(a_i^{\text{pred}} - a_i\right)$$

Order of accuracy: **2**

Iteration: multi-stage methods

The result of the LNe corrector step can be used to compute new a_i^{pred} which yield a new $u_i^{\text{L},n+1}$: Iterations inside the actual time step.

This iteration converges, but not to the analitical solution.
The order of accuracy remains **2**, but the error slightly decreases.



The optimal version is LNe3

Third order 3-stage methods

- The order of accuracy can be increased only be fractional time steps

CCL method:

1. **C**Ne formula 1/3 length time step
2. **C**Ne formula 2/3 length time step
3. **L**Ne formula full-length time step

CLL módszer:

1. **C**Ne formula 2/3 length time step
2. **L**Ne formula 2/3 length time step
3. **L**Ne formula full-length time step

The Quadratic-neighbour (CLQ) method

- The ODE system:

$$\frac{du_i(t)}{dt} = -2\frac{r}{h}u_i(t) + \underbrace{\frac{r}{h}u_{i\pm1}(t) + q_i}_{w_i t^2 + s_i t + a_i}$$

We want a polynomial with degree 3: we need function values in 3 points:

In the beginning, the middle and the end of the time step.

Half and full steps

Predictor steps: CNe and LNe formulas.

The CLQ algorithm

- 1. Full-length CNe: $u_i^{\mathrm{C}} = u_i^n e^{-2r} + A_i\left(1 - e^{-2r}\right)$ where $A_i = \frac{u_{\mathrm{i}\pm1}^{\mathrm{n}}}{2} + \frac{h}{2r} q_i$
- 2. Full and half length LNe using $A_i^{\mathrm{pred}} = \frac{u_{i\pm1}^{\mathrm{C}}}{2} + \frac{h}{2r} q_i$
- 3. The result:

$$u_i^{\mathrm{Q}} = e^{-2r} u_i^{\mathrm{n}} + \left(1 - e^{-2r}\right)\left(\frac{W_i}{2r^2} - \frac{S_i}{2r} + A_i\right) + W_i\left(1 - \frac{1}{r}\right) + S_i$$

- Where

$$F_{1,i} = \frac{u_{i\pm1}^{L\frac{1}{2}}}{2} + \frac{h}{2r} q_i \qquad F_{2,i} = \frac{u_{i\pm1}^{L}}{2} + \frac{h}{2r} q_i$$

$$S_i = 4F_{1,i} - F_{2,i} - 3A_i \qquad W_i = 2\left(F_{2,i} - 2F_{1,i} + A_i\right)$$

- Order of accuracy: **3**

Iteration: multi-stage CLQ(n) methods

- The result of the Q corrector step can be sed to calculate new a_i^{pred}

With this we can perform new corrector steps inside the time step.

For this, we need to compute the solution in the middle of the time step:

$$u_i^{Q1/2} = e^{-r} u_i^n + \left(1 - e^{-r}\right)\left(\frac{W_i}{2r^2} - \frac{S_i}{2r} + A_i\right) + \frac{W_i}{4} - \frac{W_i}{2r} + \frac{S_i}{2}$$

- 4 stage: CLQ2, Order of accuracy: **4**

5 and 6 stage: CLQ3 and CLQ4: still fourth order

CLQ5 and above: no unconditional stability

If we omit the LNe phase, we obtain **CQ**(n) :

Little bit more accurate, but **no** unconditional stability.

Pseudo-implicit approach

Θ-formula:

$$\frac{dy}{dt} = f(t,y) \quad \rightarrow \quad \frac{y^{n+1} - y^{n}}{\Delta t} = \theta f\left(t^{n}, y^{n}\right) + (1-\theta)\, f\left(t^{n+1}, y^{n+1}\right)$$

For the heat equation:

$$\frac{u_i^{n+1} - u_i^{n}}{\Delta t} = \frac{\alpha}{\Delta x^2}\left[\theta\left(u_{i-1}^{n} - 2u_i^{n} + u_{i+1}^{n}\right) + (1-\theta)\left(u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}\right)\right]$$

Trick: the **neighbours** are treated **fully explicitely**,

but the actual *u* is partialy **implicitely** (pseudo-implicit trick).

$$\frac{u_i^{n+1} - u_i^{n}}{\Delta t} = \frac{\alpha}{\Delta x^2}\left[\theta\left(u_{i-1}^{n} - 2u_i^{n} + u_{i+1}^{n}\right) + (1-\theta)\left(u_{i-1}^{n} - 2u_i^{n+1} + u_{i+1}^{n}\right)\right]$$

The new u_i^{n+1} values can be explicitely expressed!

Pseudo-implicit approach

$$\frac{u_i^{n+1}-u_i^n}{\Delta t}=\frac{\alpha}{\Delta x^2}\left[\theta\left(u_{i-1}^n-2u_i^n+u_{i+1}^n\right)+(1-\theta)\left(u_{i-1}^n-2u_i^{n+1}+u_{i+1}^n\right)\right]$$

Example: ***θ=1/2***

$$\frac{u_i^{n+1}-u_i^n}{\Delta t}=\frac{\alpha}{\Delta x^2}\left[\left(u_{i-1}^n+u_{i+1}^n\right)+\frac{1}{2}\left(-2u_i^n\right)+\frac{1}{2}\left(-2u_i^{n+1}\right)\right]$$

$$u_i^{n+1}=\frac{(1-r)u_i^n+r\left(u_{i-1}^n+u_{i+1}^n\right)}{1+r} \qquad r=\frac{\alpha h}{\Delta x^2}$$

The denominator is positive and the mesh ratio r in the denominator helps stability

Pseudo-implicit approach: UPFD method

$$\frac{u_i^{n+1}-u_i^{n}}{\Delta t}=\frac{\alpha}{\Delta x^2}\left[\theta\left(u_{i-1}^{n}-2u_i^{n}+u_{i+1}^{n}\right)+(1-\theta)\left(u_{i-1}^{n}-2u_i^{n+1}+u_{i+1}^{n}\right)\right]$$

Example: ***θ=0***

$$u_i^{n+1}=\frac{u_i^n+r\left(u_{i-1}^n+u_{i+1}^n\right)}{1+2r}$$

Unconditionally Positive Finite Difference (UPFD) method

Designed for the linear diffusion-convection-reaction PDE by Chen-Charpentier and Kojouharov, 2013

- 1 stage, order of accuracy: **1**

Pseudo-implicit *method*

2-stage version to reach order of accuracy: **2**

First stage: ***θ=0,*** *half time step*

$$u_i^{\text{pred}} = \frac{u_i^n + r/2\left(u_{i-1}^n + u_{i+1}^n\right)}{1+r}$$

Second stage, ***θ=1/2,*** full time step:

$$u_i^{n+1} = \frac{(1-r)u_i^n + r\left(u_{i-1}^{\text{pred}} + u_{i+1}^{\text{pred}}\right)}{1+r}$$

Odd-even hopscotch methods

- Spatial domain is divided into odd-even cells
- First compute u for all odd cells, then for the even cells
- Always the latest values are used.
- Original version (OOEH):

  First stage: Explicit Euler

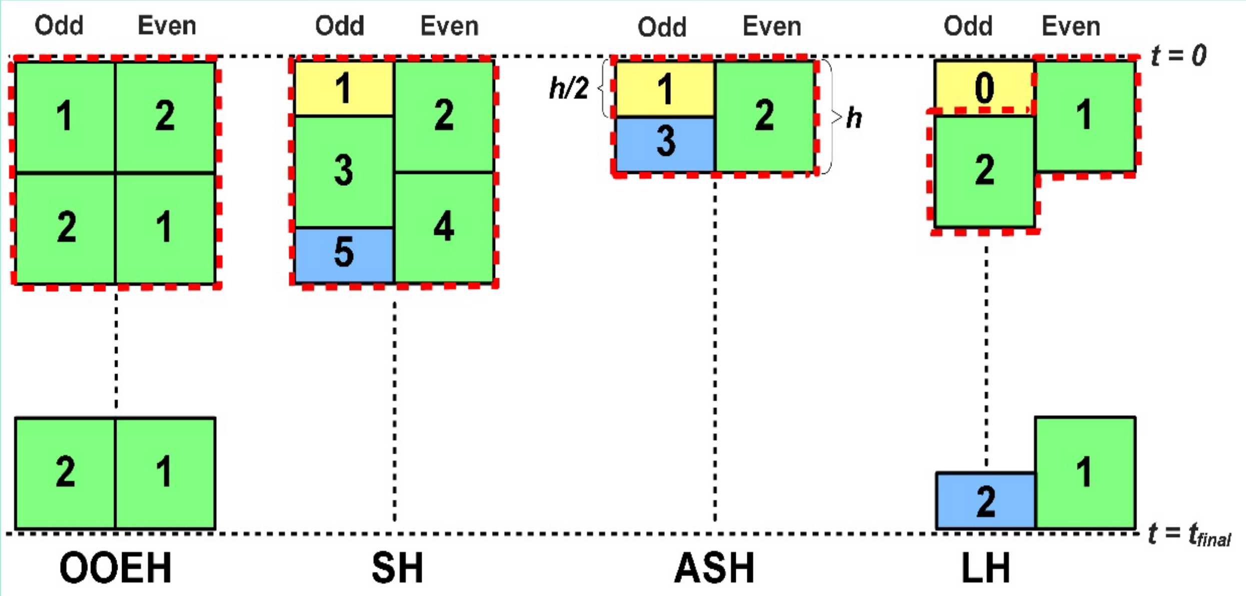
  Second stage: Implicit Euler (made fully explicit)

Order of accuracy: **2**

First we tried to change the formulas:

1. Reverse the order (UPFD + Explicit Euler) Reversed hopscotch method
2. Use the CNe formula

Odd-even hopscotch methods



- Idea: shift the odd and even compared to each other
- The latest neighbor values are used, optimal case: **middle** of the time step $u_{i\pm1}^{n+1/2}$
- What formulas should be used?

We tried a large number (up to 100000) combination, obtained a few optimal case.

The SH and ASH methods

Psedo-implicit approach, θ formula.

Shifted-hopscotch (SH):

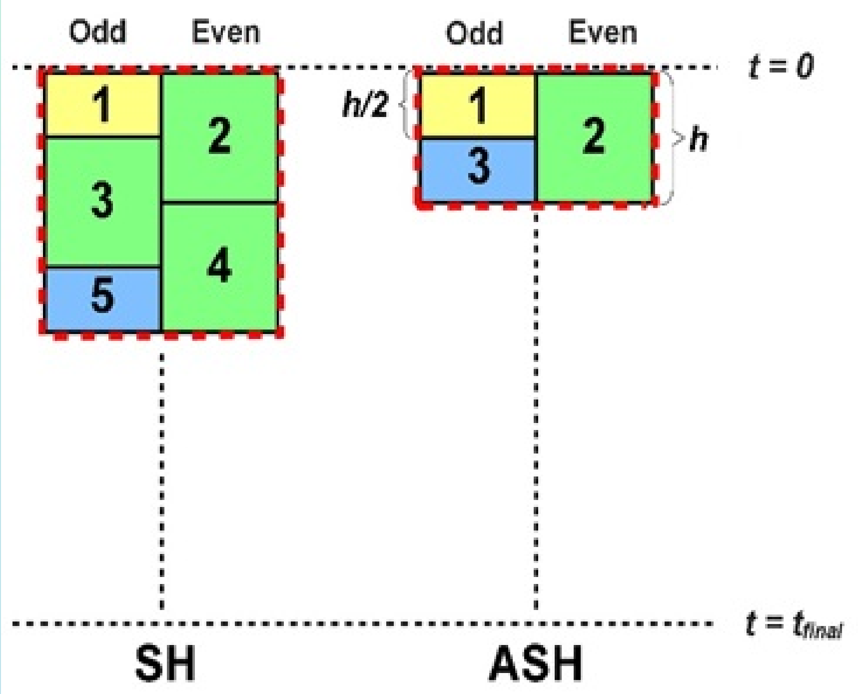
- Stage 1: half length, $\theta=0$
- Stages 2-3-4: full length, $\theta=1/2$

$$u_i^n = \frac{(1-r)u_i^{n-1} + r\left(u_{i-1}^{n-1/2} + u_{i+1}^{n-1/2}\right) + hq_i}{1+r}$$

- Last stage: half length, $\theta=1$

Assymetric-hopscotch (ASH):

- Same, but two stages are omitted



The Leapfrog-Hopscotch (LH) method

Psedo-implicit approach, θ formula.

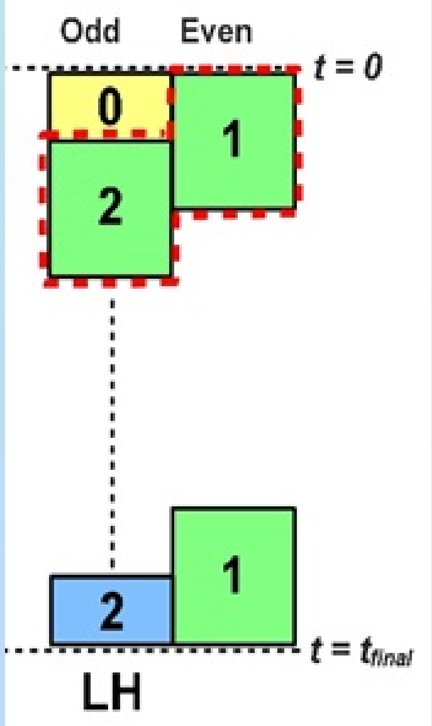
- Stage 0: half length, $\theta=0$

$$u_i^{1/2} = \frac{u_i^0 + r/2\left(u_{i-1}^0 + u_{i+1}^0\right) + h/2 \cdot q_i}{1+r}$$

- Further stages: full length, $\theta=1/2$

$$u_i^n = \frac{(1-r)u_i^{n-1} + r\left(u_{i-1}^{n-1/2} + u_{i+1}^{n-1/2}\right) + hq_i}{1+r}$$

- Last stage: half length, $\theta=1/2$ $\quad r \to r/2$

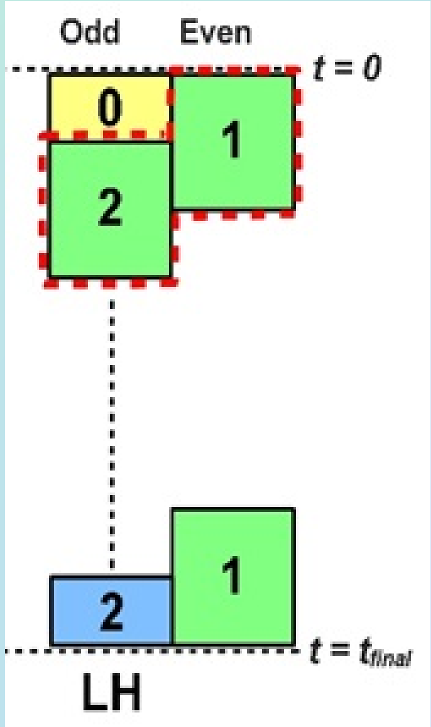


A Leapfrog-Hopscotch-CNe (LH-CNe) method

The **Constant-neighbour** formula is used in each stage.

First half, then a lot of integer,

then finally a half time step



Already known explicit stable methods

- UPFD
- Original odd-even hopscotch (OOEH)
- Dufort-Frankel
- Alternating Direction Explicit (ADE)
- Rational Runge-Kuta (RRK)

Generalization: resistance-capacitance model

- If the material properties are space-dependent,
- and/or the geometry is more complicated.

Cell-capacity: $C_i = c_i \rho_i V_i$ Resistance: $R_{ij} = d_{ij} / k_{ij} A_{ij}$

ODE system:

$$\frac{du_i}{dt} = \sum_{j \neq i} \frac{u_j - u_i}{R_{i,j} C_i} + q_i$$

Lumped parameter thermal network (LPTN)

In a matrix form:

$$\frac{d\vec{u}}{dt} = M\vec{u} + \vec{q}$$

Generalization: RC model

$$\frac{d\vec{u}}{dt} = M\vec{u} + \vec{q} \qquad \frac{du_i}{dt} = \sum_{j \neq i} \frac{u_j - u_i}{R_{i,j} C_i} + q_i$$

Example: The general version of the CNe formula:

$$u_i^{n+1} = e^{-r_i} u_i^n + \left(1 - e^{-r_i}\right) \cdot h a_i / r_i$$

where $r_i = -h m_{ii}$.

Contains only the matrix-elements:

the methods can be applied to other ODE systems

Analytical results: convex combination property

- **We proved that when the CNe, LNe(n), CpC, LH-CNe methods are applied to the general equation**

$$\frac{du_i}{dt} = \sum_{j \neq i} \frac{u_j - u_i}{R_{i,j} C_i}$$

Then the new u_i^{n+1} **values are the** convex combination **of the old ones** u_j^n **(thus the initial ones).**

- **The same is proven for the CLQ - CLQ(n), n<5 methods, if they are applied for the simplest equation**

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

This implies **unconditional stability** and the Second Law of Thermodynamics.

Analytical results: unconditional stability

- **We proved that the CCL, CLL, PI and LH methods are unconditionally stable when applied to the simple diffusion equation**

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

Proof: von-Neumann method for the PI, CCL and CLL,

The eigenvalues of the matrix of two stages for the LH.

Analytical results: accuracy for ODEs

- **We proved that if applied to the**

$$\frac{d\vec{u}}{dt} = M\vec{u} + \vec{Q} \qquad \vec{u}(t=0) = \vec{u}^0$$

Initial value problem, the orders of temporal convergence are the following:

1 CNe

2 LNe(n), CpC

3 CCL, CLL, CLQ

4 CLQ2, CLQ3 and CLQ4

This implies the order of convergence in the time step size for the spatially discretized diffusion equation in arbitrary dimensions and mesh type/size

(for the **Lumped parameter thermal network LPTN**)

Analytical results: accuracy for special ODEs

We proved that if applied to the ODE system or initial value problem

$$\frac{du_i}{dt} = \alpha \frac{u_{i-1} - 2u_i + u_{i+1}}{\Delta x^2} \qquad \vec{u}(t=0) = \vec{u}^0$$

obtained by the spatial discretization of the diffusion equation, the order of temporal convergence is 2 **for the PI, LH and LH-CNe methods.**

Proof: Calculation of the local errors for the **ODE** system

PI: generalized to the case with the linear convection term

Analytical results: local truncation errors

We calculated the local truncation errors for Eq. $\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$

Examples:

$$\tau_{CNe} = \tau_{CDF} + \alpha^2 u_{(2x)} \boxed{\frac{\Delta t}{\Delta x^2}} + \frac{7}{12}\alpha^2 u_{(4x)} \Delta t + \frac{\alpha^2}{360} u_{(6x)} \Delta x^2 \Delta t - \frac{2}{3}\alpha^3 u_{(2x)} \boxed{\frac{\Delta t^2}{\Delta x^4}} - \frac{\alpha^3}{18} u_{(4x)} \boxed{\frac{\Delta t^2}{\Delta x^2}} + \frac{89}{540}\alpha^3 u_{(6x)} \Delta t^2 + \ldots$$

Terms reflect inconsistency

$$\tau_{\mathrm{LH}} = \tau_{\mathrm{CDF}} + \frac{\alpha^3}{4} u_{(4x)} \boxed{\frac{\Delta t^2}{\Delta x^2}} + \frac{\alpha^3}{24} u_{(6x)} \Delta t^2 + \ldots$$

Nonlinear equations: Fisher and Huxley

Operator-splitting:

The method handling the diffusion term gives a „predictor” $\left(u_i^{\text{pred}}\right)$

Then the increment due to the nonlinear term is taken into account in the corrector-step.

Fisher

$$\beta u(1-u) = \beta u - \beta uu$$

Huxley

$$\beta u^2(1-u) = \beta u^2 - \beta u^2 u$$

Substitution: $u \to u_i^{\text{pred}}$ or u_i^{n+1}

$$u_i^{n+1} = u_i^{\text{pred}} + \beta h\left(u_i^{\text{pred}} - u_i^{\text{pred}} u_i^{n+1}\right)$$

$$u_i^{n+1} = u_i^{\text{pred}} + \beta h\left\{\left(u_i^{\text{pred}}\right)^2 - \left(u_i^{\text{pred}}\right)^2 u_i^{n+1}\right\}$$

$$u_i^{\text{n+1}} = \frac{1+\beta h}{1+\beta h u_i^{\text{pred}}} u_i^{\text{pred}}$$

$$u_i^{\text{n+1}} = \frac{1+\beta h u_i^{\text{pred}}}{1+\beta h\left(u_i^{\text{pred}}\right)^2} u_i^{\text{pred}}$$

These can be combined with Strang-splitting.

Analytical results: dynamical consistency

- **We proved that if the formulas above are combined with the previously mentioned convex combination methods, the obtained operator-splitting methods are dynamically consistent for the Fisher and Huxley euqations, thus the solution remains in the [0,1] interval if the initial function has values in this [0,1] interval.**
- **Similar statement is proven in a wide parameter region for the Nagumo-equation.**
- This guarantees stability for arbitrary time step size and nonlinear coefficient.

1. Numerical case study

- Linear diffusion-equation
- The diffusion coefficient depend on space: $\alpha(x) = \bar{\alpha} x^m$

  which means $\frac{\partial u(x,t)}{\partial t} = \bar{\alpha} \frac{\partial}{\partial x}\left(x^m \frac{\partial u(x,t)}{\partial x} \right)$

The analytical solution:

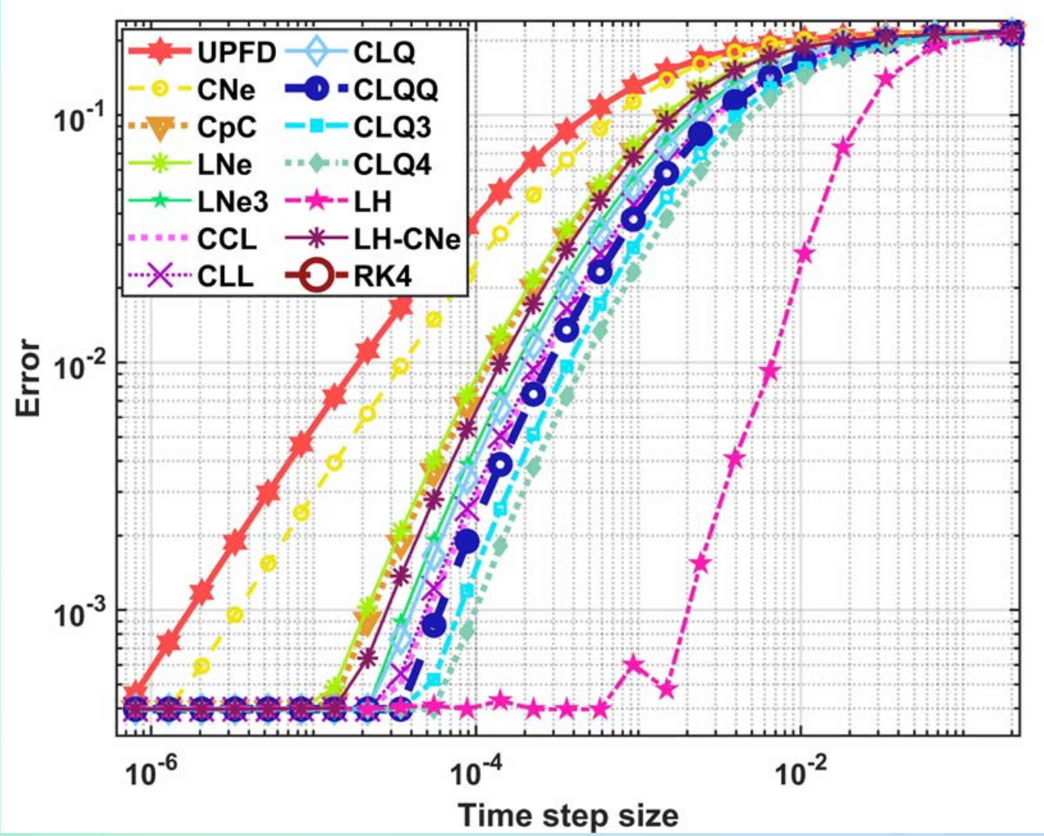
$$u(x,t) = t^{-\frac{3}{2}} f\left(\frac{x}{t^\beta}\right) = \sqrt{\frac{t^{\beta-3}}{x}} \cdot e^{-\frac{\left(\frac{x}{t^\beta}\right)^{-m+2}}{2(m-2)^2}} \cdot M_{\frac{(1+3(m-2))|m-2|}{2(m-2)^2}, \frac{m-1}{2m-4}}\left(\frac{|m-2|\left(\frac{x}{t^\beta}\right)^{-m+2}}{(m-2)^3} \right)$$

M: Kummer-function

RC model, space-dependent *R*-s

1. Numerical case study

$$\alpha(x) = \bar{\alpha}\, x^m \quad m = 20,\ N = 299,\ \Delta x = 2\cdot 10^{-3} \quad \Rightarrow\ h_{\mathrm{MAX}}^{\mathrm{EE}} = 6.3\times 10^{-8}$$



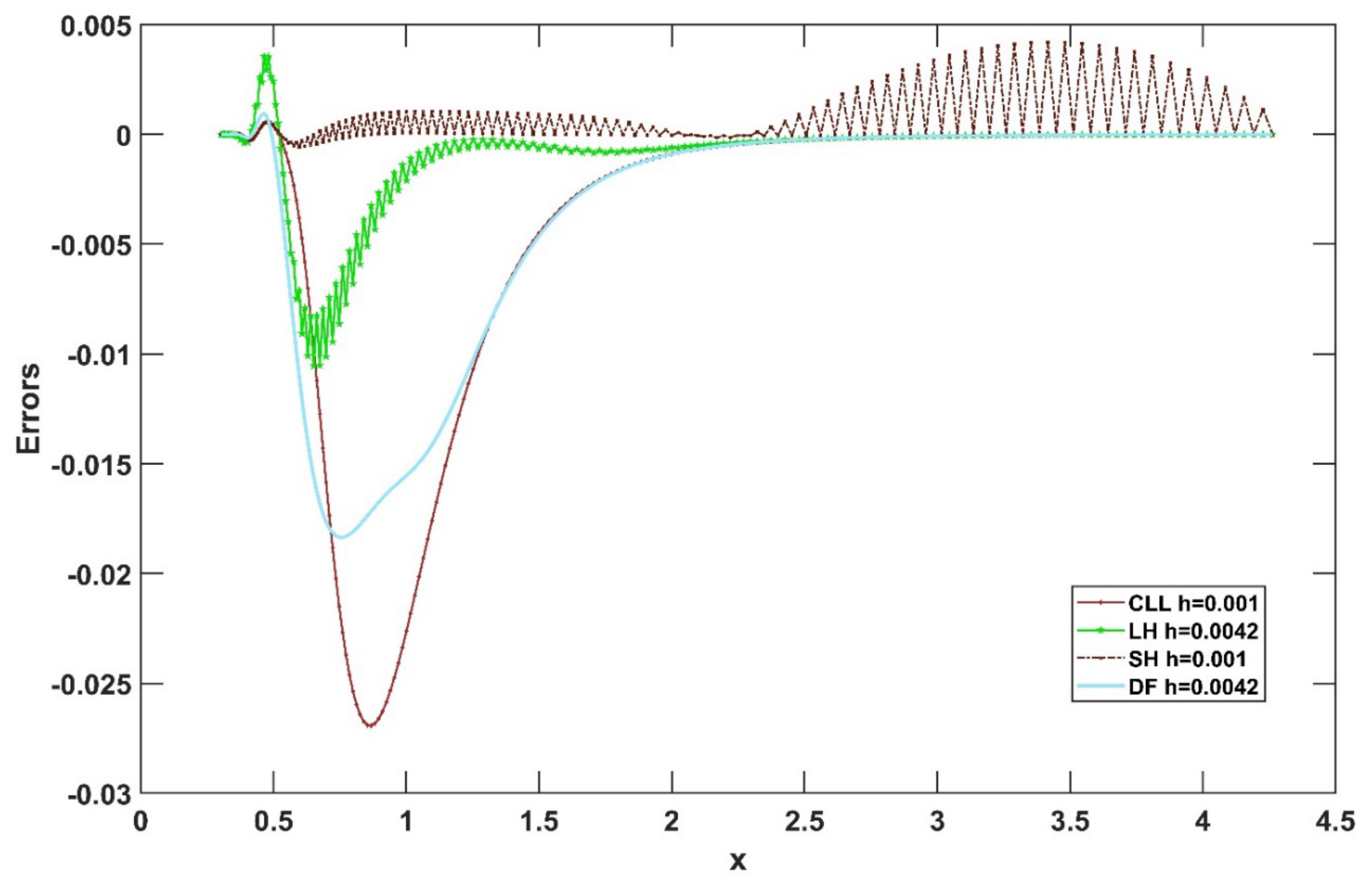
If N is increased to $N = 799$: $h_{\mathrm{MAX}}^{\mathrm{EE}} = 5.6\times 10^{-14}$, RK methods do not work.

Can non-physical **oscillations emerge**?

Convex combination methods: **never** for the linear heat equation

Example: very stiff system,

$$h_{MAX}^{FTCS} = 2.3 \cdot 10^{-8}$$



2. Numerical case study

- Linear diffusion-equation
- The diffusion coefficient depend on **space and time**:

$$\alpha(x,t)=\bar{\alpha}\left(\frac{x}{\sqrt{t}}\right)^m$$

which means

$$\frac{\partial u(x,t)}{\partial t}=\bar{\alpha}\frac{\partial}{\partial x}\left(\left(\frac{x}{\sqrt{t}}\right)^m\frac{\partial u(x,t)}{\partial x}\right)$$

The analytical solution:

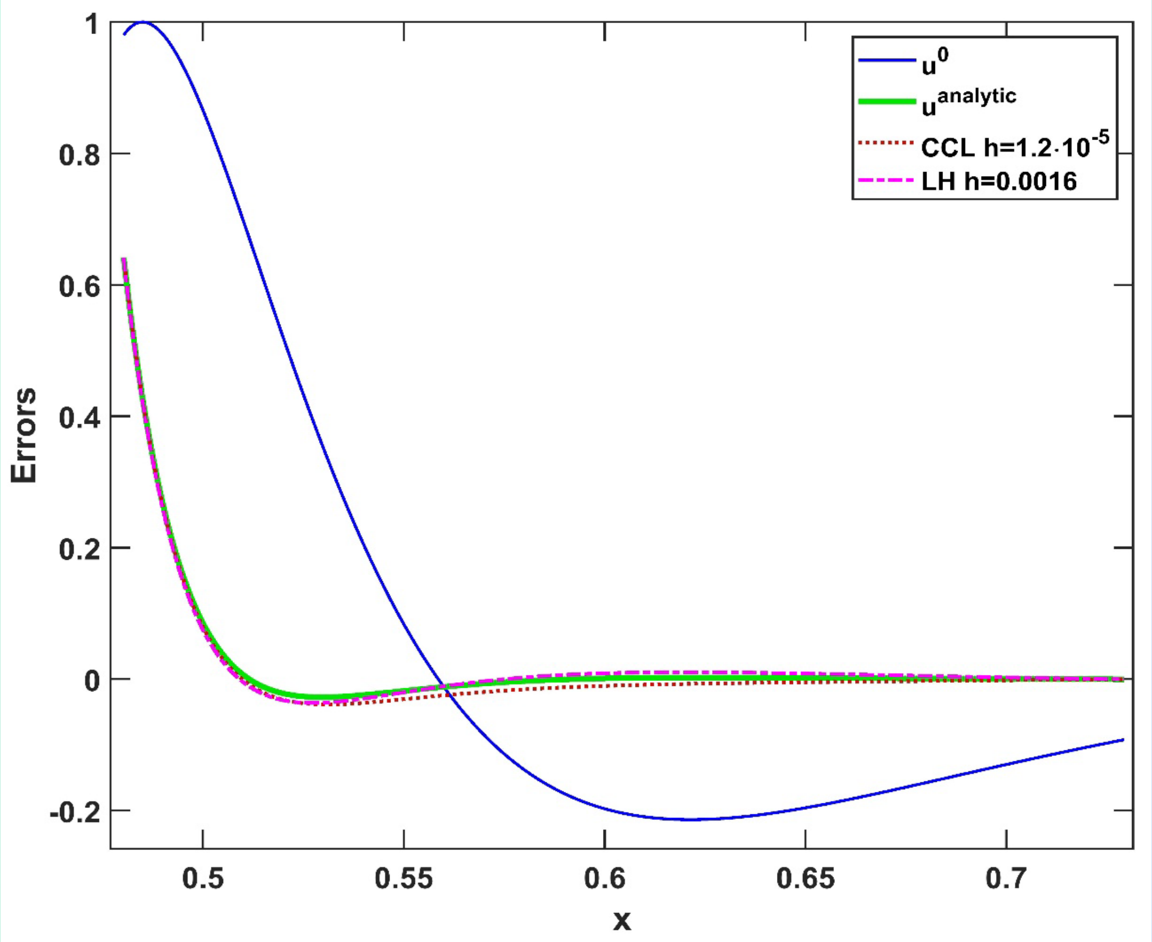
$$u(x,t)=t^{-\alpha}f\left(\frac{x}{t^{\beta}}\right)=c_2\sqrt{\frac{t^{1/2-2\alpha}}{x}}\cdot e^{\frac{\left(x/\sqrt{t}\right)^{2-m}}{4(m-2)}}\cdot W_{\frac{4\alpha-1}{2m-4},\frac{m-1}{2m-4}}\left(\frac{\left(x/\sqrt{t}\right)^{2-m}}{2(m-2)}\right)$$

W: Whittaker-function

RC model, space and time-dependent *R*-s

2. Numerical case study

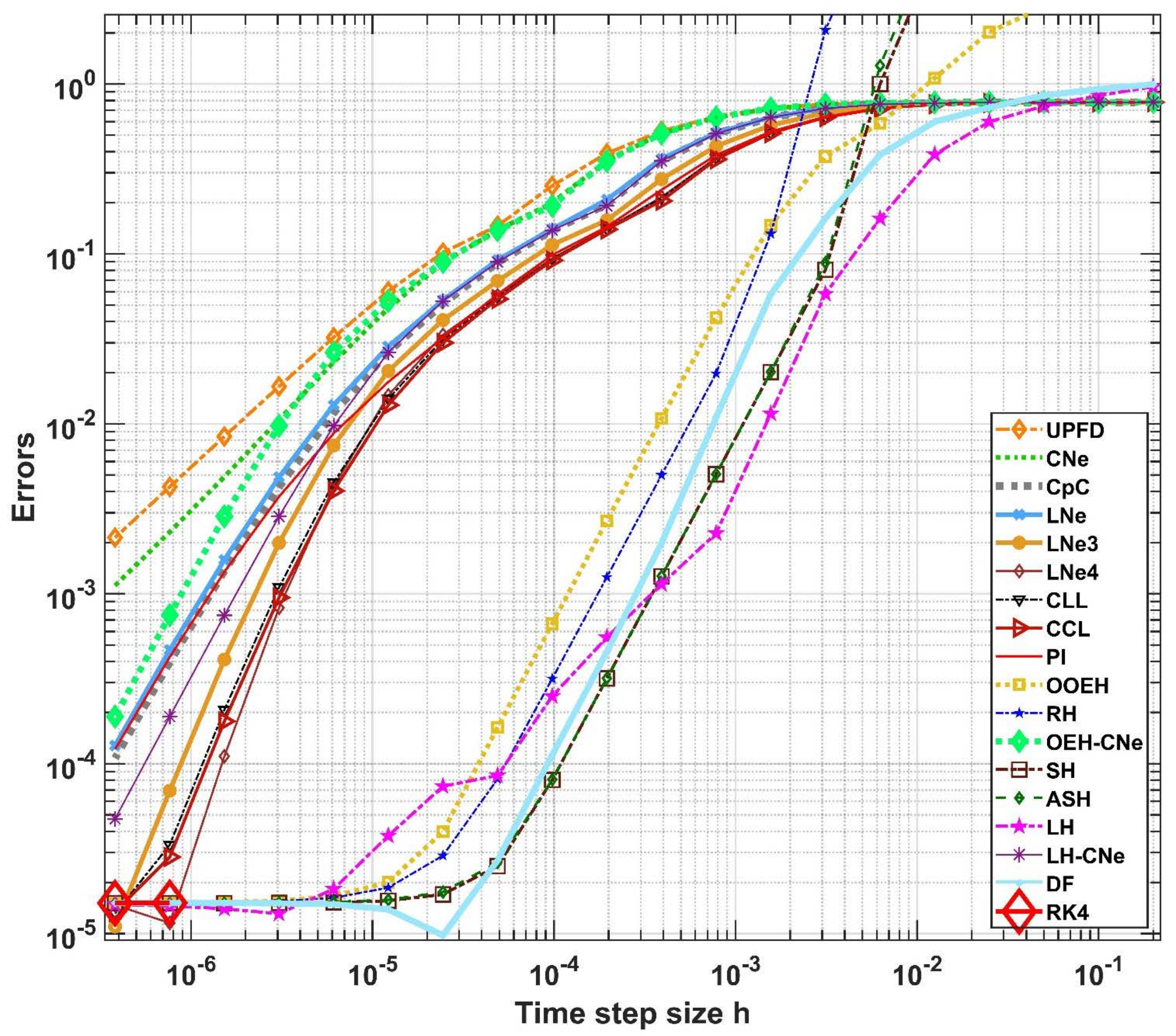
$$\alpha(x,t)=\bar{\alpha}\left(\frac{x}{\sqrt{t}}\right)^m \qquad m=7.2\,,\ \Delta x=5\cdot 10^{-4} \qquad h_{CFL}^{EE}\left(t^0\right)=8.65\cdot 10^{-7} \rightarrow h_{CFL}^{EE}\left(t^{\text{fin}}\right)=5.44\cdot 10^{-6}$$



2. Numerical case study

$$\alpha(x,t) = \bar{\alpha}\left(\frac{x}{\sqrt{t}}\right)^m$$

$$h_{CFL}^{EE} \approx 10^{-6}$$

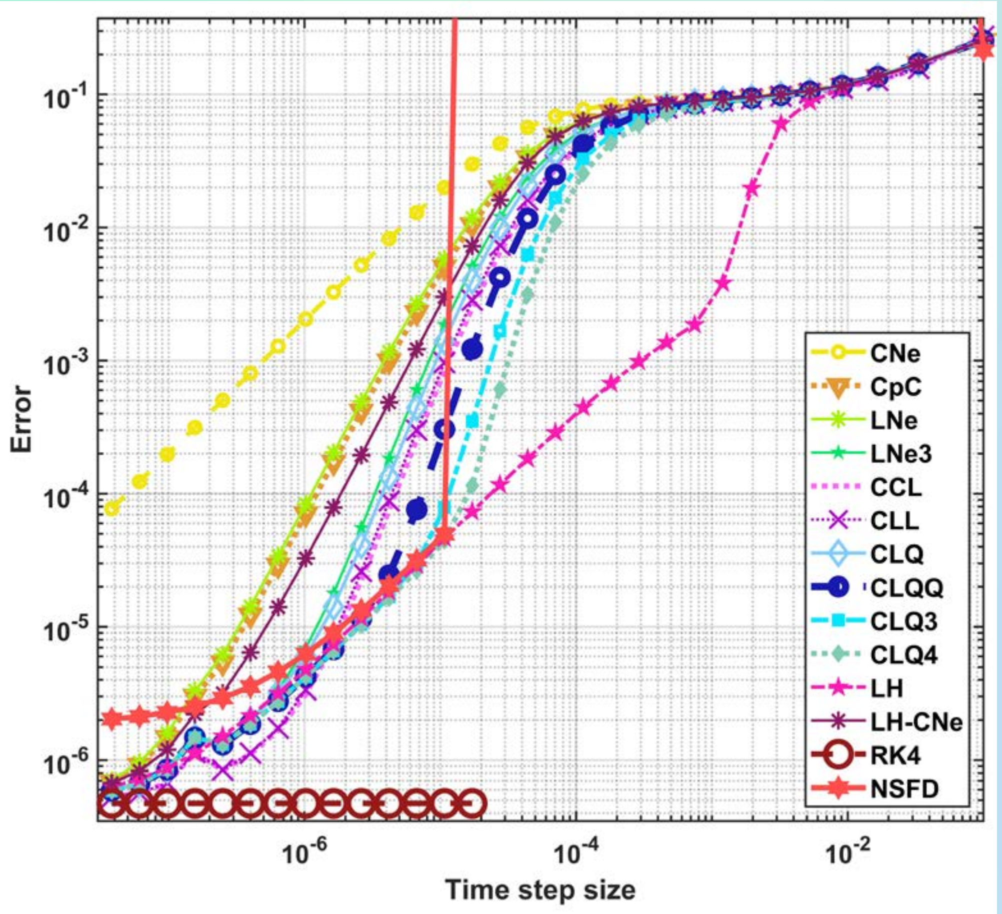


3. Numerical case study: Fisher-equation

$\alpha = 1, \beta = 20$

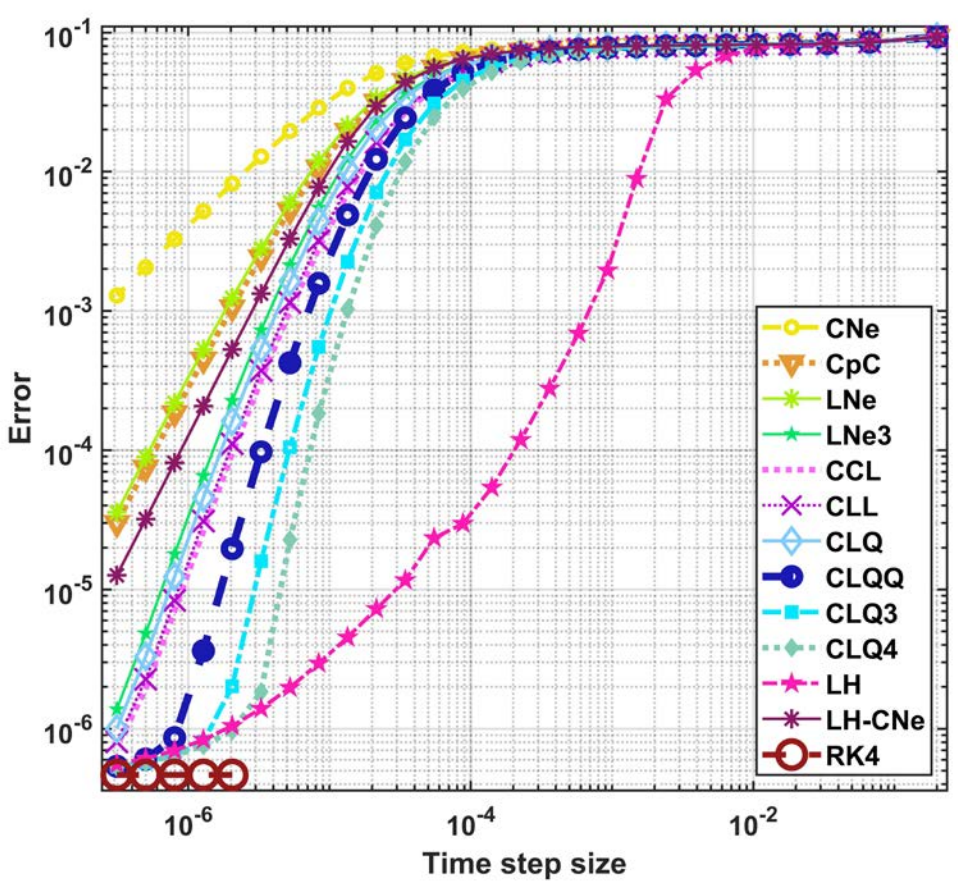
Analitical solution:

$$u^{\text{exact}}(x,t) = \left(1 + e^{\sqrt{\frac{\beta}{6}}x - \frac{5}{6}\beta t}\right)^{-2}$$



4. Numerical case study: Huxley-equation

$\alpha = 1, \beta = 7$ Analitical solution: $u^{\text{exact}}(x,t) = \dfrac{e^{bx+b^2t}}{c + e^{bx+b^2t}}$ where $b = \sqrt{\dfrac{b}{2}}$



5. Numerical case study: Huxley-equation

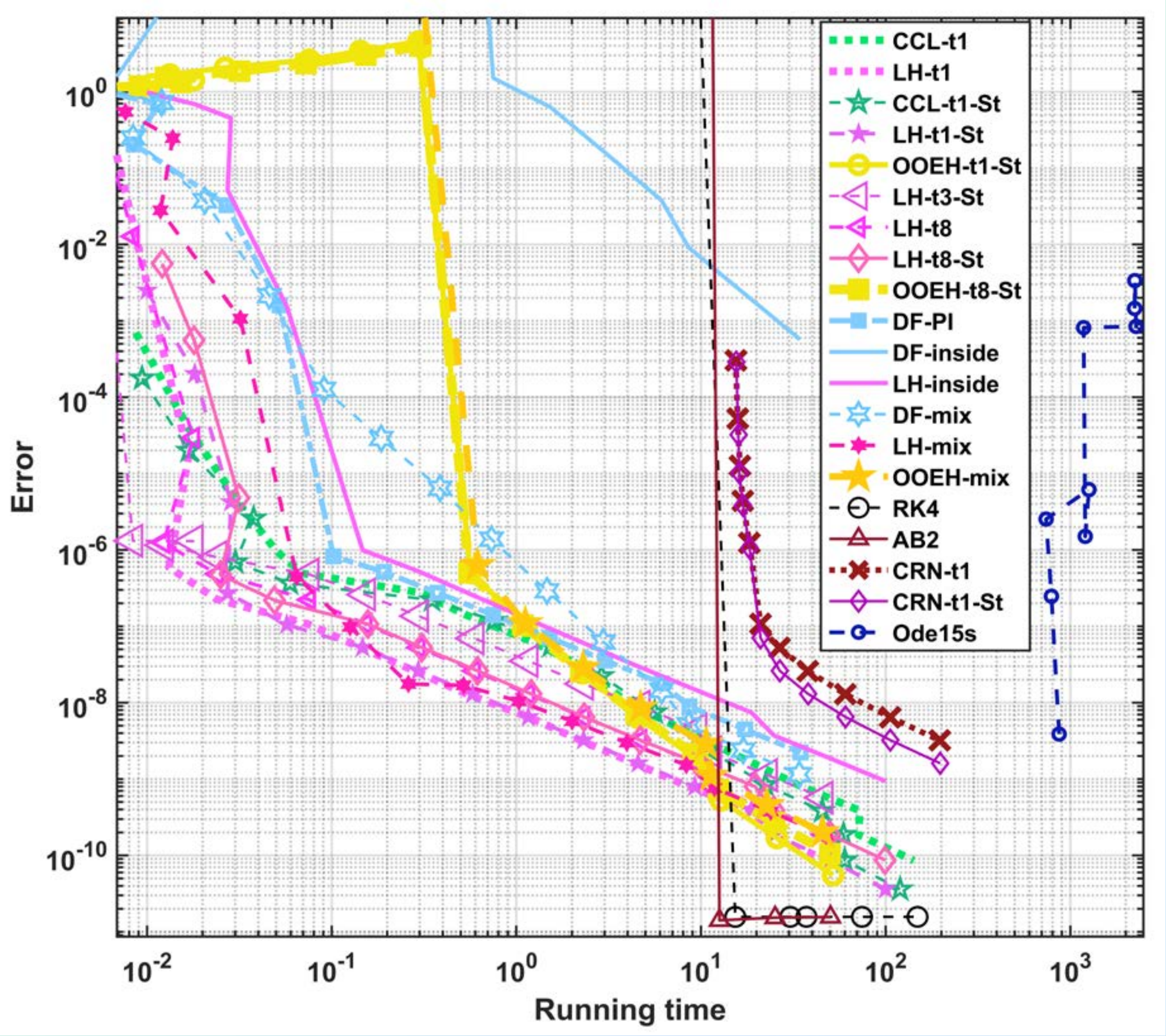
2D $N = N_x \times N_y = 101 \times 120 = 12120$ $\alpha = 1$, $\beta = 21$

RC model,

random *R* and *C* values,

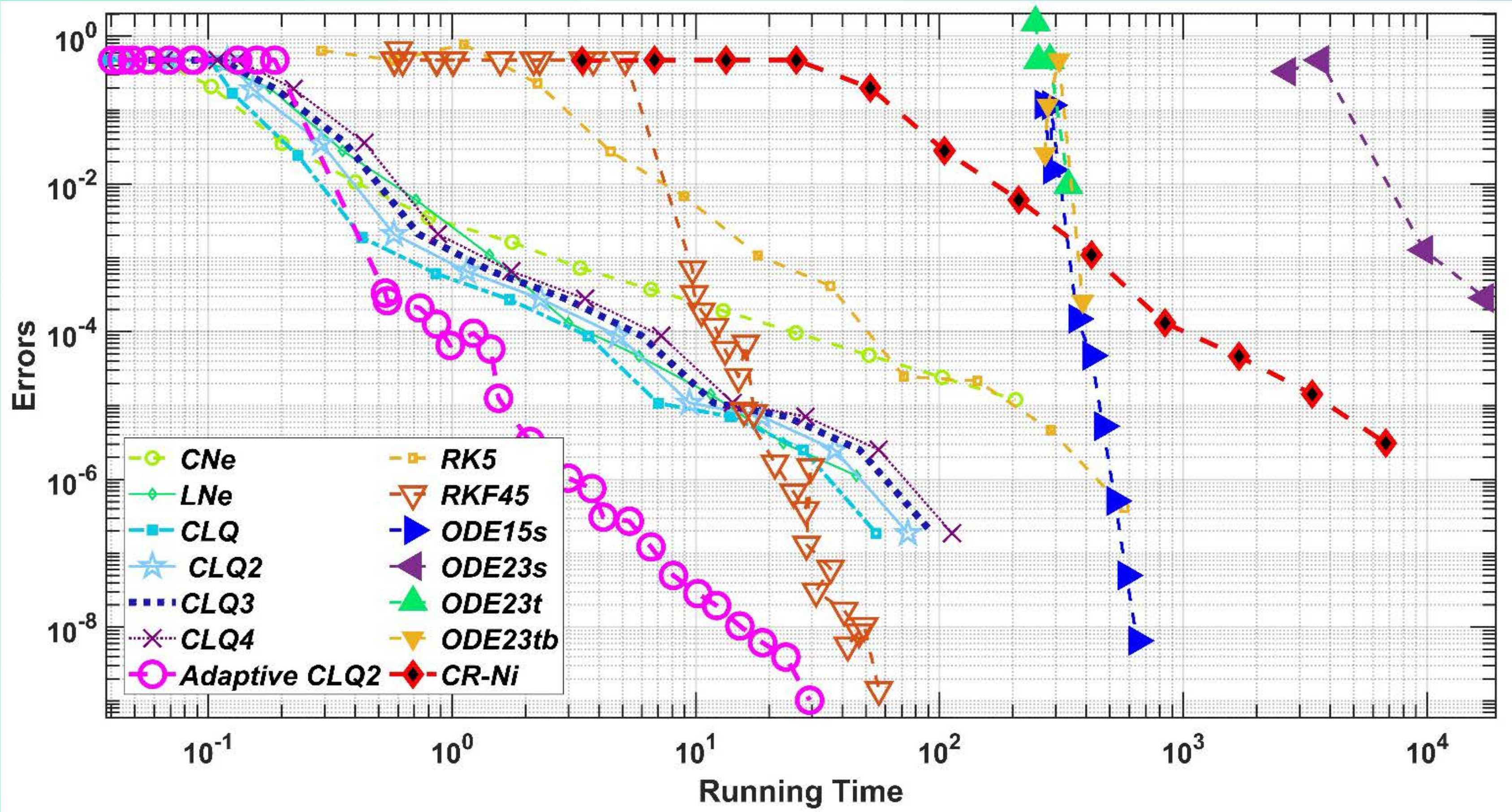
$SR = 8.6 \cdot 10^5$, $h_{\text{MAX}}^{\text{EE}} = 7 \cdot 10^{-5}$

Numerical reference solution



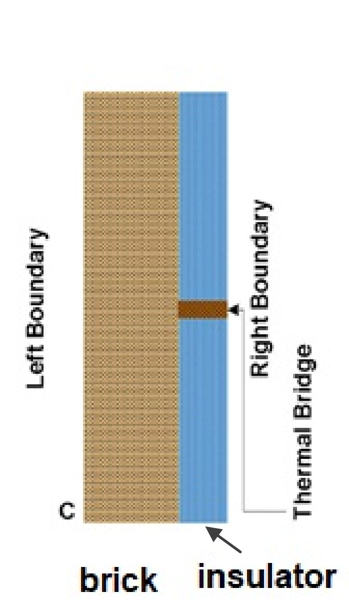
6. Numerical case study

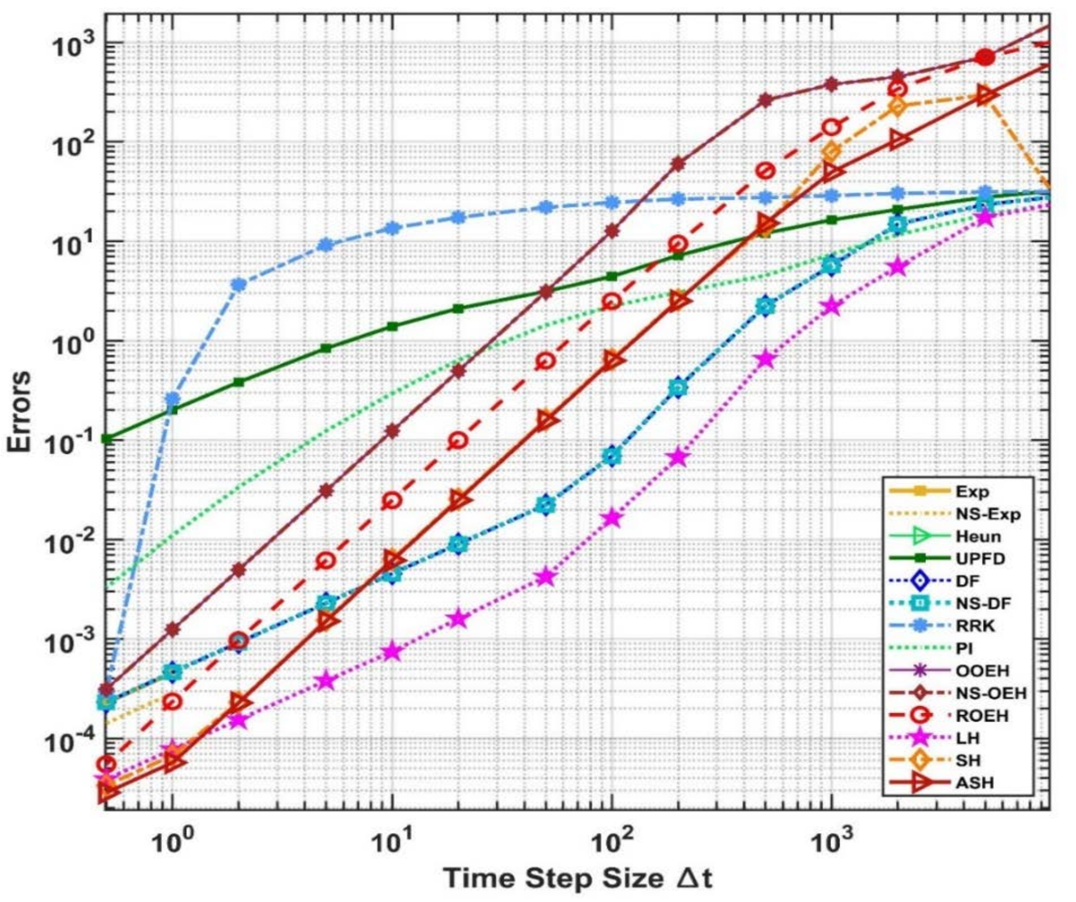
Heat conduction with random initial conditions and moving and pulsing heat source, 2D, $N = N_x \times N_y = 100 \times 100 = 10\,000$



7. Numerical case study: Wall with a thermal bridge

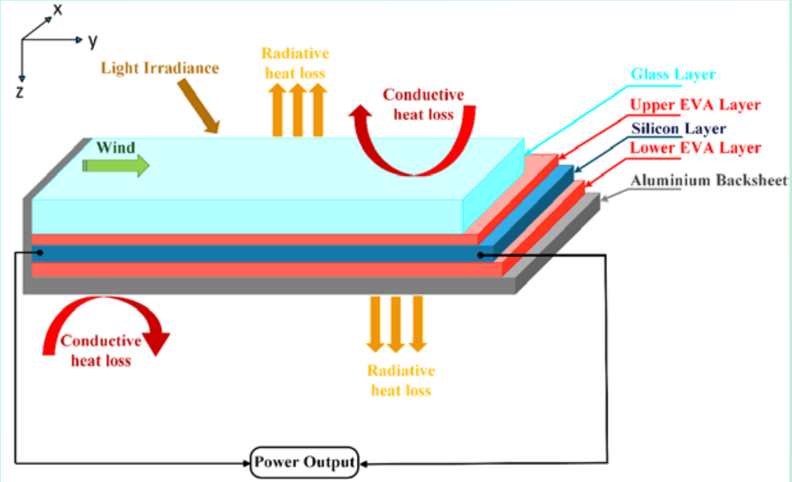
2D heat transfer with material inhomogeneity

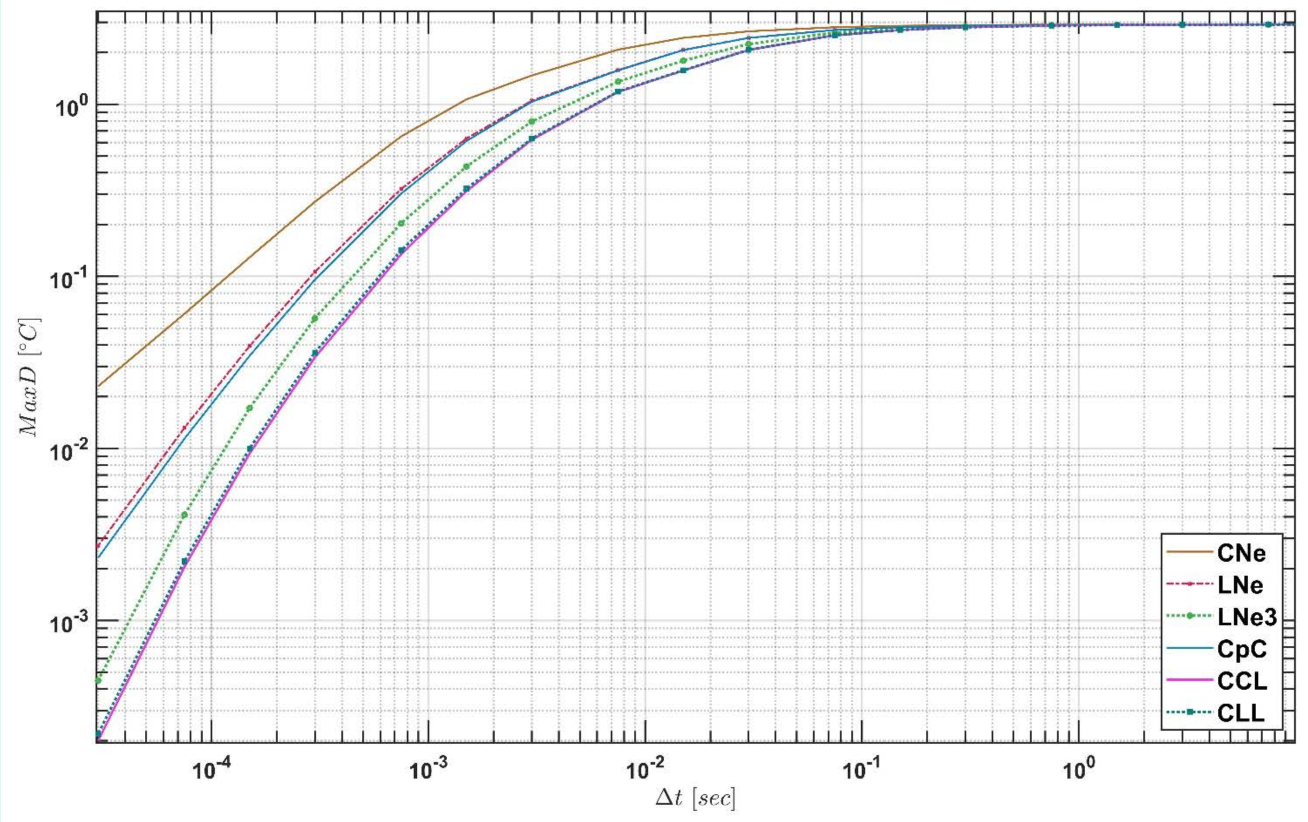




8. Numerical case study: 3D solar panel

heat transfer with several types of heat source





Conclusions

The methods have been applied to several problems.

Based on a large number of numerical case studies,

- the proposed algorithms are competitive compared to the traditional algorithms in the case of low or medium accuracy requirements.
- Their advantage compared to the standard **explicit** methods increases with the inhomogeneity of the media or the irregularity of the spatial mesh.
- Their advantage compared to the standard **implicit** methods increases with the size of the spatial mesh.
- The **LH** is almost always the most efficient (less inconsistent terms in the truncation error)

Closely related publications

[1] E. Kovács, “New Stable, Explicit, First Order Method to Solve the Heat Conduction Equation,” J. Comput. Appl. Mech., vol. 15, no. 1, pp. 3–13, 2020.

[2] E. Kovács, Á. Nagy, and M. Saleh, “A set of new stable, explicit, second order schemes for the non-stationary heat conduction equation,” Mathematics, vol. 9, no. 18, p. 2284, Sep. 2021. **Q2**

[3] E. Kovács, “A class of new stable, explicit methods to solve the non-stationary heat equation,” Numer. Methods Partial Differ. Equ., vol. 37, no. 3, pp. 2469–2489, 2020 **Q1**

[4] E. Kovács and Á. Nagy, “A new stable, explicit, and generic third-order method for simulating conductive heat transfer,” Numer. Methods Partial Differ. Equ., vol. 39, no. 2, pp. 1504–1528, Nov. 2023. **Q1**

[5] E. Kovács, Á. Nagy, and M. Saleh, “A New Stable, Explicit, Third-Order Method for Diffusion-Type Problems,” Adv. Theory Simulations, 2022, **Q1**

[6] Á. Nagy, I. Omle, H. Kareem, E. Kovács, I. F. Barna, and G. Bognar, “Stable, Explicit, Leapfrog-Hopscotch Algorithms for the Diffusion Equation,” Computation, vol. 9, no. 8, p. 92, 2021. **Q2**

[7] A. H. Askar, Á. Nagy, I. F. Barna, and E. Kovács, “Analytical and Numerical Results for the Diffusion-Reaction Equation When the Reaction Coefficient Depends on Simultaneously the Space and Time Coordinates,” Comput. 2023, Vol. 11, Page 127, vol. 11, no. 7, p. 127, Jun. 2023. **Q2**

[8] E. Kovács, J. Majár and M. Saleh, “Unconditionally positive, explicit, fourth order method for the diffusion- and Nagumo-type diffusion-reaction equations”, accepted for publication in Journal of Scientific Computing. **D1**

Other related publications (Q1)

The methods have been applied to several problems

[9] E. Kovács et al. „Analytical and numerical study of diffusion propelled surface growth phenomena” Partial Diff. Eqs in Applied Mathematics 11 Paper: 100798 , 10 p. (2024) (**KPZ** equation)

[10] M. Saleh, E. Kovács, N. Kallur, “Adaptive step size controllers based on Runge-Kutta and linear-neighbor methods for solving the non-stationary heat conduction equation,” Networks Heterog. Media 2023 31059, vol. 18, no. 3, pp. 1059–1082, 2023.

[11] H. K. Jalghaf, I. Omle, E. Kovács, „A Comparative Study of Explicit and Stable Time Integration Schemes for Heat Conduction in an Insulated Wall” BUILDINGS 12 : 6 Paper: 824 , 24 p. (2022)

[12] H. K. Jalghaf, E. Kovács, and B. Bolló, “Comparison of Old and New Stable Explicit Methods for Heat **Conduction, Convection, and Radiation in an Insulated Wall with Thermal Bridging**,” Buildings, vol. 12, no. 9, p. 1365, Sep. 2022.

[13] I. Omle, Issa ; E. Kovács; B. Bolló, „Applying recent efficient numerical methods for long-term simulations of heat transfer in walls to **optimize thermal insulation**” RESULTS IN ENG. 20 Paper: 101476 , 19 p. (2023)

[14] H. K. Jalghaf, E. Kovács, „Simulation of **phase change materials** in building walls using effective heat capacity model by recent numerical methods” J. OF ENERGY STORAGE 83 Paper: 110669 , 16 p. (2024)

[15] Á.,Nagy, I. Bodnár, E. Kovács, „Simulation of the Thermal Behavior of a **Photovoltaic Solar Panel** Using Recent Explicit Numerical Methods” ADVANCED THEORY AND SIMULATIONS 2024 Paper: 2400089 (2024)

Thank you for your kind attention!