

A fourth order stencil for parabolic PDEs under Dirichlet boundary conditions

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Some References

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Numerical Solution of Time-Dependent Advection-Diffusion-Reaction
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Berlin, 2003.
- ② [González-Pinto S. and Hernández-Abreu, D.](#)
Boundary corrections for splitting methods in the time integration of
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Scope of the talk

- ① A fourth order space discretization based on finite differences for 1D-parabolic problems
- ② Justification of the convergence order in some important norms. Illustrations
- ③ Extension to several dimensions
- ④ Work in progress

1D-Parabolic Problems (Advective form)

The 1D-version of the PDE parabolic problem is

$$\text{(PDE)} \quad u_t(x, t) = \mathcal{L}u + r(x, t, u), \quad x \in \Omega = (0, 1), \quad t \in I^* = (0, t^*],$$

$$\mathcal{L}u(x, t) = a(x, t) \partial_{xx}u + b(x, t) \partial_x u \quad (\text{Advective form})$$

$$a(x, t) \geq \bar{a} > 0, \quad (x, t) \in \Omega \times I^*$$

$$\text{(BCs)} \quad u(0, t) = \beta(0, t), \quad u(1, t) = \beta(1, t), \quad t \in I^*,$$

$$\text{(IC)} \quad u(x, 0) = g(x), \quad x \in \Omega,$$

Spatial Semidiscretization based on central differences

$$\text{(PDE)} \quad \dot{v}_j(t) = \mathcal{L}^{(h)} v_j(t) + r(x_j, t, v_j), \quad x_j = j h, \quad h = \Delta x = \frac{1}{(m+1)},$$

$$\mathcal{L}^{(h)} v_j(t) = a_j(t) \partial_{xx}^{(h)} v_j + b_j(t) \partial_x^{(h)} v_j$$

$$a_j(t) = a(x_j, t), \quad b_j(t) = b(x_j, t), \quad v_j(t) \approx u(x_j, t)$$

$$\text{(BCs)} \quad v_0(t) = \beta(0, t), \quad v_{m+1}(t) = \beta(1, t), \quad t \in I^*,$$

$$\text{(IC)} \quad v_j(0) = g(x_j), \quad j = 1, 2, \dots, m.$$

Simple fourth Order Spatial Semidiscretization

$$\mathcal{L}^{(h)} v_j(t) = a_j(t) \partial_{xx}^{(h)} v_j + b_j(t) \partial_x^{(h)} v_j$$

$$\partial_{xx}^{(h)} v_j = \begin{cases} \frac{-(v_{j-2} + v_{j+2}) + 16(v_{j-1} + v_{j+1}) - 30v_j}{12h^2}, & 2 \leq j \leq m-1 \\ \frac{v_{j-1} - 2v_j + v_{j+1}}{h^2}, & j = 1 \text{ and } j = m, \end{cases}$$
$$\partial_x^{(h)} v_j = \begin{cases} \frac{(v_{j-2} - v_{j+2}) - 8(v_{j-1} - v_{j+1})}{12h}, & 2 \leq j \leq m-1, \\ \frac{-v_{j-1} + v_{j+1}}{2h}, & j = 1 \text{ and } j = m. \end{cases}$$

$$(\mathcal{L} - \mathcal{L}^{(h)})u_j(t) = \begin{cases} \mathcal{O}(h^2), & j = 1 \text{ and } j = m \\ \mathcal{O}(h^4), & 2 \leq j \leq m-1 \end{cases}$$

Why a fourth order stencil? (Accuracy and Stiffness)

For 2D-parabolic problems in rectangular domains

$$u_t(\vec{x}, t) = \Delta u + r(\vec{x}, t, u), \quad \text{with (Dir.BCs) and (IC)}$$

- 1 The second order stencil based on central differences makes use of N^4 grid-points to get accuracy $\mathcal{O}(N^{-4})$. $\Delta x = \Delta y = N^{-2}$
- 2 The fourth order stencil makes use of N^2 grid-points to get a similar accuracy. $\Delta x = \Delta y = N^{-1}$
- 3 Additionally, the stiffness for the second option is enormously reduced and this allows time integrations with some explicit methods.

- 1 Stiffness with the second order stencil to get accuracy $\mathcal{O}(N^{-4})$

$$\lambda_{\min} \approx -\frac{4}{\Delta x^2} - \frac{4}{\Delta y^2} \approx -8 N^4, \quad \Delta x = \Delta y = N^{-2}$$

- 2 Stiffness with the fourth order stencil to get accuracy $\mathcal{O}(N^{-4})$

$$\lambda_{\min} \approx -\frac{4}{\Delta x^2} - \frac{4}{\Delta y^2} \approx -8 N^2, \quad \Delta x = \Delta y = N^{-1}$$

Why a fourth order stencil? (Accuracy and Complexity)

The time integrations of the resulting ODE with ADI-type methods involve

- 1 The solution of N^2 tridiagonal systems of dimension N^2 per integration time-step with the second order stencil.

$$\text{Accuracy} = \mathcal{O}(N^{-4}) \leftrightarrow \text{Comput Costs} = N^2 \cdot \mathcal{O}(N^2) \text{ flops/integ. step}$$

- 2 The solution of N penta-diagonal systems of dimension N per integration time-step with the fourth order stencil.

$$\text{Accuracy} = \mathcal{O}(N^{-4}) \leftrightarrow \text{Comput Costs} = N \cdot \mathcal{O}(N) \text{ flops/integ. step}$$

Positivity (TVD)

A space discretization

$$v'(t) = A(t) v(t), \quad A(t) = (a_{i,j}(t))_{1 \leq i,j \leq m}, \quad t \in I^*,$$

is positive iff

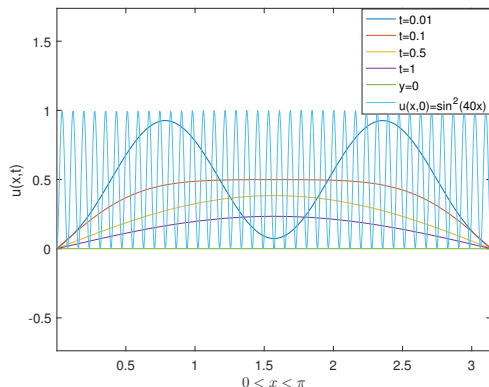
$$a_{i,j}(t) \geq 0, \quad \forall i \neq j, t \in I^*.$$

- 1 The second order stencil is positive in absence of advection.
- 2 The fourth order stencil is not positive in absence of advection.
- For parabolic problems this fact does not appear to be of major concern.
- It can be a problem for advection dominated problems with steep fronts and reaction terms.

Positivity (TVD) of the fourth order stencil

$$u_t = u_{xx}, \quad 0 < x < \pi, \quad t \in [0, 1],$$

$$u(x, 0) = \sin^2(40x), \quad u(0, t) = u(\pi, t) = 0$$



The local truncation error

- The discretized ODE

$$\dot{V}(t) = \mathcal{L}^{(h)}V + r_h(t, V) = J_h(t)V + \beta_h(t) + r_h(t, V)$$

$\beta_h(t)$ stems from the Dirichlet boundary conditions.

- The PDE solution $U(t) = (u(x_j, t))_{j=1}^m$ satisfies

$$\dot{U}(t) = \mathcal{L}U + r_h(t, U) = \mathcal{L}^{(h)}U(t) + r_h(t, U) + \sigma_h(t)$$

where $\sigma_h(t)$ represents the local truncation error. In our case

$$\sigma_h(t) = (\mathcal{L} - \mathcal{L}^{(h)})U(t)$$

- Observe that both \mathcal{L} and $\mathcal{L}^{(h)}$ include the Dirichlet BCs.

Ingredients for convergence in 1D-problems

We focus on the simplest case $\mathcal{L} = \partial_{xx}$ with Homogeneous Dirichlet BCs.

$$\sigma_h(t) := \dot{U}(t) - (D_{xx}U(t) + r(t, U)), \quad h = \Delta x = \frac{1}{m+1}$$

$$D_{xx} = \frac{1}{12h^2} \begin{pmatrix} -24 & 12 & 0 & 0 & & & & & & & 0 \\ 16 & -30 & 16 & -1 & 0 & & & & & & 0 \\ -1 & 16 & -30 & 16 & -1 & 0 & & & & & 0 \\ 0 & -1 & 16 & -30 & 16 & -1 & 0 & & & & 0 \\ \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & & & \vdots \\ \vdots & & & & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ 0 & & & & & -1 & 16 & -30 & 16 & -1 & 0 \\ 0 & & & & & & -1 & 16 & -30 & 16 & 0 \\ 0 & & & & & & & 0 & 0 & 12 & -24 \end{pmatrix}$$

Ingredients

Standard result of convergence in norms

Theorem (A)

$$\|\sigma_h(t)\| \leq C h^p; \quad \|e^{tD_{xx}}\| \leq K; \quad (t > 0, h > 0)$$

Implies

$$\|U(t) - V(t)\| \leq K^* h^p, \quad (t, h > 0)$$

But we use a refined result [Hundsdorfer-Verwer, 2003]

Theorem (B)

$$\sigma_h(t) = h^p(D_{xx}\xi(t) + \eta(t)); \quad \|\xi\|, \|\dot{\xi}\|, \|\eta\| \leq C; \quad \|e^{tD_{xx}}\| \leq K; \quad (t > 0, h > 0)$$

Implies

$$\|U(t) - V(t)\| \leq K^* h^p, \quad (t, h > 0)$$

First assumption in Theorem (B)

- The local truncation error satisfies

$$\sigma_h(t) = -\frac{h^2}{12} \left(\partial_x^4 u(x_1, t) \vec{e}_1 + \partial_x^4 u(x_m, t) \vec{e}_m \right) + \mathcal{O}(h^4)$$

- We have to express the local error as

$$\sigma_h(t) = h^4 (D_{xx} \xi_h(t) + \eta_h(t)),$$

- with bounded functions $\xi_h(t)$ and $\eta_h(t)$. This is equivalent

$$h^4 D_{xx} \xi^{(1)} = -\frac{h^2}{12} \vec{e}_1 \partial_x^4 u(x_1, t), \quad h^4 D_{xx} \xi^{(m)} = -\frac{h^2}{12} \vec{e}_m \partial_x^4 u(x_m, t).$$

- This leads to

$$\begin{aligned} \hat{D}_{xx} \xi^{(1)} &= \vec{e}_1, & \hat{D}_{xx} \xi^{(m)} &= \vec{e}_m, & \hat{D}_{xx} &= h^2 D_{xx} \\ \xi_h(t) &= -\frac{1}{12} \left(\partial_x^4 u(x_1, t) \xi^{(1)} + \partial_x^4 u(x_m, t) \xi^{(m)} \right) \end{aligned}$$

First assumption in Theorem (B)

- ① The linear equation for $\xi = \xi^{(1)}$ reads

$$-\xi_{j-2} + 16 \xi_{j-1} - 30 \xi_j + 16 \xi_{j+1} - \xi_{j+2} = 0 \quad \text{for } j = 2, \dots, m-1$$

- ② together with

$$\xi_0 = 0, \quad \xi_{m+1} = 0, \quad \xi_0 - 2\xi_1 + \xi_2 = 1, \quad \xi_{m-1} - 2\xi_m + \xi_{m+1} = 0.$$

- ③ The characteristic equation of the recurrence relation is

$$0 = \rho^4 - 16\rho^3 + 30\rho^2 - 16\rho + 1 = (\rho - 1)^2(\rho^2 - 14\rho + 1),$$

- ④ and has a double root at $\rho = 1$ and single roots at $\rho_0 = 7 - 4\sqrt{3} \approx 0.0718$ and $\rho_0^{-1} = 7 + 4\sqrt{3}$.

- ⑤ The general solution is

$$\xi_j = a + bj + c\rho_0^j + d\rho_0^{-j}.$$

First assumption in Theorem (B)

- 1 The coefficients a, b, c, d are given by

$$c = \frac{1}{(1 - \rho_0)^2(1 - \rho_0^{2m-2})}, \quad d = -c \rho_0^{2m}.$$

$$a = -\frac{(1 - \rho_0^{2m})}{(1 - \rho_0)^2(1 - \rho_0^{2m-2})}, \quad b = h \frac{(1 - \rho_0^{2m})(1 - \rho_0^{m+1})}{(1 - \rho_0)^2(1 - \rho_0^{m-1})}.$$

- 2 Since $\rho_0 = 7 - 4\sqrt{3} \approx 0.0718$ is small, we have

$$\xi_j \approx (-1 + x_j)/(1 - \rho_0)^2,$$

- 3 which is clearly bounded for $j = 0, \dots, m + 1$ and arbitrary $h = 1/(m + 1) > 0$.

Second assumption in some ℓ_p -norms

- It is well known that for any operator matrix norm $\|\cdot\|$,

$$\|e^{tA}\| \leq e^{t\mu[A]}, \quad \forall t \geq 0, \quad \mu[A] := \lim_{\epsilon \downarrow 0} \frac{\|I + \epsilon A\| - 1}{\epsilon},$$

where A is a square real matrix and $\mu[A]$ is its logarithmic "norm".

- The smallest constant satisfying $\|e^{tA}\| \leq e^{tc}$, $\forall t \geq 0$ is $c = \mu[A]$.
- For matrices $A = D_{xx}$ the norms induced by the vector weighted Euclidean norm and the Euclidean norm coincide,

$$\|V\|_{2,h}^2 = h \sum_{j=1}^m |v_j|^2 = h \|V\|_2^2$$

Theorem

$$\mu_{2,h}[D_{xx}] = \mu_2[D_{xx}] = \lambda_{\max}\left(\frac{1}{2}(D_{xx} + D_{xx}^\top)\right) < -9, \quad \forall h > 0.$$

This fact allows to apply the Theorem with constant $K = 1 = \sup_{t \geq 0} e^{-9t}$

Second assumption in some ℓ_p -norms

$h = 1/(m + 1)$	$\mu_2[D_{xx}]$	$\mu_\infty[D_{xx}]$
1/10	-9.7750	3.3333e+01
1/20	-9.8242	1.3333e+02
1/40	-9.8470	5.3333e+02
1/80	-9.8583	2.1333e+03
1/160	-9.8639	8.5333e+03
1/320	-9.8668	3.4133e+04
1/640	-9.8682	1.3653e+05
1/1280	-9.8689	5.4613e+05
1/2560	-9.8693	2.1845e+06
1/5120	-9.8694	8.7381e+06

Table: Logarithmic "norms" (euclidean and maximum norms) of the matrices D_{xx} for different values of m .

We have shown that

$$\lim_{m \rightarrow \infty} \mu_2[D_{xx}] = -\pi^2, \quad \mu_\infty[D_{xx}] = \frac{1}{3h^2}$$

Boundedness in l_∞ -norm (from the l_2 -norm)

- Recall that

$$\|U\|_{2,h} = \sqrt{h \sum_{i=1}^m |U_i|^2}, \quad \|U\|_\infty = \max_{i=1,\dots,m} |U_i|.$$

- It holds

$$\|U\|_{2,h} \leq \|U\|_\infty \leq \frac{1}{\sqrt{h}} \|U\|_{2,h}.$$

- The error

$$err_m(t) = V_m(t) - U_m(t),$$

- $V_m(t)$ is the exact solution of the m -dimensional ODE
 $U_m(t) = (u(x_j, t))_{j=1}^m$ and $u(x, t)$ is the exact solution of the PDE

$$\|err_m(t)\|_{2,h} \leq c h^4 e^{-9t}, \quad \forall h, t > 0$$

because of $\mu_{2,h}[D_{xx}] < -9$.

Consequently

$$\|err_m(t)\|_\infty \leq c h^{3.5} e^{-9t}, \quad \forall h, t > 0.$$

Additional result of convergence

Theorem

Assume $u(x, 0) = g(x) \in L^2(0, 1)$, $r(t, u) \equiv 0$. Then, for any fixed $t_0 > 0$ there exist a positive constant K_0 such that for

$$\|err_m(t)\|_\infty \leq K_0 h^4, \quad \forall h > 0, t \geq t_0.$$

Some numerical examples

PDE model

$$u_t(x, t) = u_{xx}; \quad u(0, t) = u(1, t) = 0; \quad u(0, x) = g(x); \quad t > 0, \quad 0 < x < 1.$$

Exact PDE solution is given by

$$u(x, t) = \sum_{n=1}^{\infty} \alpha_n e^{-(n\pi)^2 t} \sin n\pi x, \quad \alpha_n = 2 \int_0^1 g(x) \sin n\pi x dx.$$

1 $g(x) = 4x(1 - x), \quad u(x, t) = \left(\frac{2}{\pi}\right)^3 \sum_{n=1}^{\infty} \frac{1+(-1)^{n+1}}{n^3} e^{-(n\pi)^2 t} \sin n\pi x$

2
$$\begin{cases} g(x) = 1 \quad (0 < x < 1), & g(0) = g(1) = 0 \\ u(x, t) = \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1+(-1)^{n+1}}{n} e^{-(n\pi)^2 t} \sin n\pi x \end{cases}$$

Some numerical examples. Example 1

$h = 1/(m + 1)$	$\ err_m(t^*)\ _{2,h}$		$\ err_m(t^*)\ _{\infty}$	
1/5	0.47129E-05		0.62571E-05	
1/10	0.19372E-06	24.32	0.26934E-06	23.23
1/20	0.84376E-08	22.95	0.11777E-07	22.87
1/40	0.40496E-09	20.83	0.56775E-09	20.74
1/80	0.21403E-10	18.92	0.30114E-10	18.85
1/160	0.12147E-11	17.62	0.17130E-11	17.57
1/320	0.72045E-13	16.86	0.10174E-12	16.83
1/640	0.43742E-14	16.47	0.61817E-14	16.45

Table: Euclidean and maximum norm of the errors, ODE solution minus PDE solution, at time $t^* = 1$, for different values of m and the initial function given by $g(x) = 4x(1 - x)$.

Some numerical examples. Example 2

$h = 1/(m + 1)$	$\ err_m(T)\ _{2,h}$		$\ err_m(T)\ _\infty$	
1/5	0.52044E-05		0.69002E-05	
1/10	0.21711E-06	23.97	0.30134E-06	22.89
1/20	0.95542E-08	22.72	0.13319E-07	22.62
1/40	0.46293E-09	20.63	0.64856E-09	20.53
1/80	0.24645E-10	18.78	0.34662E-10	18.71
1/160	0.14053E-11	17.53	0.19814E-11	17.49
1/320	0.83595E-13	16.81	0.11804E-12	16.78
1/640	0.51007E-14	16.38	0.72025E-14	16.38

Table: Euclidean and maximum norm of the errors, ODE solution minus PDE solution, at time $T = 1$, for different values of m and the initial function given by $g(x) = 1$ (discontinuous at the border).

Convergence in 2D-PDEs. A simple 2D-case

- We focus on the simplest case $\mathcal{L} = \partial_{xx} + \partial_{yy}$ with Dirichlet BCs.

$$\begin{aligned}u_t(x, y, t) &= u_{xx} + u_{yy}, & (x, y) \in \Omega \equiv (0, 1)^2, & t \in (0, t^*], \\u(x, y, t) &= \beta(x, y, t), & (x, y) \in \partial\Omega, & t \in (0, t^*], \\u(x, y, 0) &= g(x, y), & (x, y) \in \Omega.\end{aligned}$$

- In this case the spatial operator is $\mathcal{L}^{(h)} = \partial_{xx}^{(h)} + \partial_{yy}^{(h)} + \beta^{(h)}(t)$

$$\dot{W} = \mathcal{L}^{(h)} W \equiv (\mathbf{D}_{xx} + \mathbf{D}_{yy}) W + \beta^{(h)}(t), \quad W(0) = U(0), \quad t \in (0, t^*]$$

- where

$$\mathbf{D}_{xx} = I_{m_y} \otimes D_{xx}, \quad \mathbf{D}_{yy} = D_{yy} \otimes I_{m_x},$$

$$W_{i,j}(t) \simeq U_{i,j}(t) = u(x_i, y_j, t),$$

$$x_i = i\Delta x, \quad y_j = j\Delta y; \quad \Delta x = \frac{1}{m_x+1}, \quad \Delta y = \frac{1}{m_y+1}$$

Convergence in 2D-PDEs. A simple 2D-case

- We cannot apply the convergence Hundsdorfer-Verwer theorem (B), in spite of the fact that the second assumption is satisfied

$$\|e^{t(\mathbf{D}_{xx} + \mathbf{D}_{yy})}\|_2 = \|e^{t\mathbf{D}_{xx}} e^{t\mathbf{D}_{yy}}\|_2 \leq \|e^{t\mathbf{D}_{xx}}\|_2 \cdot \|e^{t\mathbf{D}_{yy}}\|_2 \leq e^{-18t}, \quad t > 0,$$

- the first assumption is violated in case of non-homogeneous Dirichlet BCs (consider $\Delta x = \Delta y = h$)

$$\begin{aligned} \sigma_h(t) &= (\partial_{xx} - \mathbf{D}_{xx})U + (\partial_{yy} - \mathbf{D}_{yy})U = h^4((\mathbf{D}_{xx} + \mathbf{D}_{yy})\xi_h(t) + \eta_h(t)) \\ &\|\xi_h(t)\|_2 \neq \mathcal{O}(1) \quad \text{or} \quad \|\eta_h(t)\|_2 \neq \mathcal{O}(1). \end{aligned}$$

Extension to several dimensions. From 1D to 2D PDEs

- We consider 3 problems and Dirichlet BCs to apply 1D-results:

$$(P_1) \quad \dot{U} = \partial_{xx} U + \partial_{yy} U + \beta^{(h)}(t), \quad U(0) = (g(x_i, y_j; 0))_{i,j},$$

$$(P_2) \quad \dot{V} = \mathbf{D}_{xx} V + \partial_{yy} U + \beta^{(h)}(t), \quad V(0) = U(0),$$

$$(P_3) \quad \dot{W} = \mathbf{D}_{xx} W + \mathbf{D}_{yy} W + \beta^{(h)}(t), \quad W(0) = U(0)$$

- The local truncation error of (P_2) regarding (P_1) is

$$\sigma_{\Delta x}(t) = (\partial_{xx} - \mathbf{D}_{xx})U = \Delta x^4(\mathbf{D}_{xx}\xi_1(t, \Delta x) + \eta_1(t, \Delta x))$$

- From the 1D-results, for each y , we have that

$$V(\cdot, y, t) - U(\cdot, y, t) = \Delta x^4 \psi_1(\cdot, y, t), \quad \psi_1(\cdot, y, t) = \mathcal{O}(1)$$

- Then

$$V(t) - U(t) = \Delta x^4 \Psi_1(t), \quad \Psi_1(t) = (\psi_1(\cdot, y_j, t))_{j=1:n} = \mathcal{O}(1)$$

Extension to several dimensions. From 1D to 2D PDEs

- By inserting this in (P_2)

$$(P_2) \quad \dot{V} = \mathbf{D}_{xx} V + \partial_{yy} V + \beta^{(h)}(t) - \Delta x^4 \partial_{yy} \Psi_1(t), \quad V(0) = U(0)$$

$$(P_3) \quad \dot{W} = \mathbf{D}_{xx} W + \mathbf{D}_{yy} W + \beta^{(h)}(t), \quad W(0) = U(0)$$

- The local truncation error of (P_3) regarding (P_2) is

$$\begin{aligned} \sigma_{\Delta y}(t) &= (\partial_{yy} - \mathbf{D}_{yy})V - \Delta x^4 \partial_{yy} \Psi_1(t) = \\ &= (\partial_{yy} - \mathbf{D}_{yy})(U + \Delta x^4 \Psi_1(t)) - \Delta x^4 \partial_{yy} \Psi_1(t) = \\ &= \Delta y^4 (\mathbf{D}_{yy} \xi_2(t) + \eta_2(t)) - \Delta x^4 \mathbf{D}_{yy} \Psi_1(t) \end{aligned}$$

- From 1D-results (by using that all, $\xi_2(t), \eta_2(t), \Psi_1(t) = \mathcal{O}(1)$)

$$W(t) - V(t) = \mathcal{O}(\Delta y^4) + \mathcal{O}(\Delta x^4)$$

- From the results above

$$W(t) - U(t) = (W(t) - V(t)) + (V(t) - U(t)) = \mathcal{O}(\Delta y^4) + \mathcal{O}(\Delta x^4) \quad \square$$

- 1 To get additional convergence results in the Maximum norm, particularly for non-homogeneous Dirichlet BCs ($a(x) > 0$)

$$u_t = a(x) u_{xx} + b(x) u_x + r(x, t), \quad (\text{Advective form})$$

and

$$u_t = (a(x) u_x)_x + (b(x) u)_x + r(x, t), \quad (\text{Conservative form})$$

- 2 To extend the results to the mD -case with a mild reaction term.
- 3 Extension to the case of parabolic problems with mixed derivatives in hyper-rectangles. Applications in Finance (Heston Model).