VERY HIGH-ORDER TIME SCHEME FOR THE FINITE VOLUME METHOD

G.J. Machado[1] S. Clain[1,2]

[1]Universidade do Minho, CMAT, *Campus* de Azurém, Guimarães, Portugal

[2]Université Paul Sabatier, Institut de Mathématique de Toulouse, Toulouse, France

SHARK-FV 2014
Ofir, 28 April – 2 May, 2014, Portugal

This research was financed by FEDER Funds through Programa Operacional Fatores de Competitividade — COMPETE and by Portuguese Funds through FCT — Fundação para a Ciência e a Tecnologia, within the Projects PEst-C/MAT/UI0013/2011 and PTDC/MAT/121185/2010

STEADY-STATE CASE

- steady-state 1D convection-diffusion equation ($\Omega =]0,1[$)

$$(v\phi)' - (\kappa\phi')' = f, \quad \text{in } \Omega$$

- boundary conditions ($\bar{x}$ is a boundary point):
  - Dirichlet: $\phi(\bar{x}) = \phi_{\mathrm{D}}(\bar{x})$
  - Neumann: $v(\bar{x})\phi(\bar{x}) - \kappa(\bar{x})\phi'(\bar{x}) = \phi_{\mathrm{T}}(\bar{x})$
- unknown $\phi : [0,1] \to \mathbb{R}$
- data (regular)
  - diffusion coefficient $\kappa : [0,1] \to \mathbb{R}^+$
  - convection coefficient (=velocity) $v : [0,1] \to \mathbb{R}$
  - source $f : [0,1] \to \mathbb{R}$
  - boundary functions: ϕ_{D}, ϕ_{T}, ϕ_{P}

STEADY-STATE CASE

- steady-state 1D convection-diffusion equation ($\Omega =]0,1[$)

$$(v\phi)' - (\kappa\phi')' = f, \quad \text{in } \Omega$$

- boundary conditions ($\bar{x}$ is a boundary point):
  - Dirichlet: $\phi(\bar{x}) = \phi_{\mathrm{D}}(\bar{x})$
  - Neumann: $v(\bar{x})\phi(\bar{x}) - \kappa(\bar{x})\phi'(\bar{x}) = \phi_{\mathrm{T}}(\bar{x})$
- unknown $\phi : [0,1] \to \mathbb{R}$
- data (regular)
  - diffusion coefficient $\kappa : [0,1] \to \mathbb{R}^+$
  - convection coefficient (=velocity) $v : [0,1] \to \mathbb{R}$
  - source $f : [0,1] \to \mathbb{R}$
  - boundary functions: ϕ_{D}, ϕ_{T}, ϕ_{P}

STEADY-STATE CASE

- steady-state 1D convection-diffusion equation ($\Omega =]0,1[$)

$$(v\phi)' - (\kappa\phi')' = f, \quad \text{in } \Omega$$

- boundary conditions ($\bar{x}$ is a boundary point):
  - Dirichlet: $\phi(\bar{x}) = \phi_{\mathrm{D}}(\bar{x})$
  - Neumann: $v(\bar{x})\phi(\bar{x}) - \kappa(\bar{x})\phi'(\bar{x}) = \phi_{\mathrm{T}}(\bar{x})$
- unknown $\phi : [0,1] \to \mathbb{R}$
- data (regular)
  - diffusion coefficient $\kappa : [0,1] \to \mathbb{R}^+$
  - convection coefficient (=velocity) $v : [0,1] \to \mathbb{R}$
  - source $f : [0,1] \to \mathbb{R}$
  - boundary functions: ϕ_{D}, ϕ_{T}, ϕ_{P}

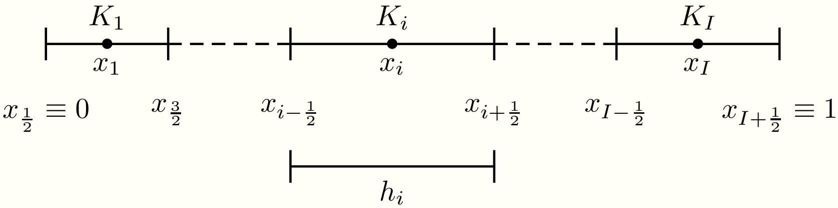
STEADY-STATE CASE

- steady-state 1D convection-diffusion equation ($\Omega =]0,1[$)

$$(v\phi)' - (\kappa\phi')' = f, \quad \text{in } \Omega$$

- boundary conditions ($\bar{x}$ is a boundary point):
  - Dirichlet: $\phi(\bar{x}) = \phi_{\mathrm{D}}(\bar{x})$
  - Neumann: $v(\bar{x})\phi(\bar{x}) - \kappa(\bar{x})\phi'(\bar{x}) = \phi_{\mathrm{T}}(\bar{x})$
- unknown $\phi : [0,1] \to \mathbb{R}$
- data (regular)
  - diffusion coefficient $\kappa : [0,1] \to \mathbb{R}^+$
  - convection coefficient (=velocity) $v : [0,1] \to \mathbb{R}$
  - source $f : [0,1] \to \mathbb{R}$
  - boundary functions: ϕ_{D}, ϕ_{T}, ϕ_{P}

NOTATION



- K_i — cell i
- I — number of cells
- $x_{i-\frac{1}{2}}$, $x_{i+\frac{1}{2}}$ — boundary points of cell i
- h_i — length of cell i
- x_i — centroid of cell i

FVM

- FV formulation

$$\frac{1}{h_i}\left(F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}\right) - \bar{f}_i = 0, i = 1, \ldots, I$$

$F_{i\pm\frac{1}{2}} = v(x_{i\pm\frac{1}{2}})\phi(x_{i\pm\frac{1}{2}}) - \kappa(x_{i\pm\frac{1}{2}})\phi'(x_{i\pm\frac{1}{2}}), \bar{f}_i = \frac{1}{h_i}\int_{K_i} f(\xi)\,\mathrm{d}\xi$

- goal — to compute an approximation to the mean value of ϕ in each cell of the mesh: $\phi_i \approx \frac{1}{h_i}\int_{K_i}\phi\,\mathrm{d}x$
- the approximation to the mean value of f over cell K_i, $f_i \approx \frac{1}{h_i}\int_{K_i} f\,\mathrm{d}x$, will be computed by gaussian quadrature
- the way that the numerical diffusive and convective fluxes are computed characterize the FVM scheme
- how to approximate numerically the fluxes with very-high precision $\mathcal{F}_{i\pm\frac{1}{2}} \approx F_{i\pm\frac{1}{2}}$: polynomial reconstructions

FVM

- FV formulation

$$\frac{1}{h_i}\left(F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}\right) - \bar{f}_i = 0, i = 1, \ldots, I$$

$F_{i\pm\frac{1}{2}} = v(x_{i\pm\frac{1}{2}})\phi(x_{i\pm\frac{1}{2}}) - \kappa(x_{i\pm\frac{1}{2}})\phi'(x_{i\pm\frac{1}{2}}), \bar{f}_i = \frac{1}{h_i}\int_{K_i} f(\xi)\,\mathrm{d}\xi$

- goal — to compute an approximation to the mean value of ϕ in each cell of the mesh: $\phi_i \approx \frac{1}{h_i}\int_{K_i} \phi\,\mathrm{d}x$
- the approximation to the mean value of f over cell K_i, $f_i \approx \frac{1}{h_i}\int_{K_i} f\,\mathrm{d}x$, will be computed by gaussian quadrature
- the way that the numerical diffusive and convective fluxes are computed characterize the FVM scheme
- how to approximate numerically the fluxes with very-high precision $\mathcal{F}_{i\pm\frac{1}{2}} \approx F_{i\pm\frac{1}{2}}$: polynomial reconstructions

FVM

- FV formulation

$$\frac{1}{h_i}\left(F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}\right) - \bar{f}_i = 0, i = 1, \ldots, I$$

$F_{i\pm\frac{1}{2}} = v(x_{i\pm\frac{1}{2}})\phi(x_{i\pm\frac{1}{2}}) - \kappa(x_{i\pm\frac{1}{2}})\phi'(x_{i\pm\frac{1}{2}}), \bar{f}_i = \frac{1}{h_i}\int_{K_i} f(\xi)\,\mathrm{d}\xi$

- goal — to compute an approximation to the mean value of ϕ in each cell of the mesh: $\phi_i \approx \frac{1}{h_i}\int_{K_i} \phi\,\mathrm{d}x$
- the approximation to the mean value of f over cell K_i, $f_i \approx \frac{1}{h_i}\int_{K_i} f\,\mathrm{d}x$, will be computed by gaussian quadrature
- the way that the numerical diffusive and convective fluxes are computed characterize the FVM scheme
- how to approximate numerically the fluxes with very-high precision $\mathcal{F}_{i\pm\frac{1}{2}} \approx F_{i\pm\frac{1}{2}}$: polynomial reconstructions

FVM

- FV formulation

$$\frac{1}{h_i}\left(F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}\right) - \bar{f}_i = 0, i = 1, \ldots, I$$

$F_{i\pm\frac{1}{2}} = v(x_{i\pm\frac{1}{2}})\phi(x_{i\pm\frac{1}{2}}) - \kappa(x_{i\pm\frac{1}{2}})\phi'(x_{i\pm\frac{1}{2}}), \bar{f}_i = \frac{1}{h_i}\int_{K_i} f(\xi)\,\mathrm{d}\xi$

- goal — to compute an approximation to the mean value of ϕ in each cell of the mesh: $\phi_i \approx \frac{1}{h_i}\int_{K_i}\phi\,\mathrm{d}x$
- the approximation to the mean value of f over cell K_i, $f_i \approx \frac{1}{h_i}\int_{K_i} f\,\mathrm{d}x$, will be computed by gaussian quadrature
- the way that the numerical diffusive and convective fluxes are computed characterize the FVM scheme
- how to approximate numerically the fluxes with very-high precision $\mathcal{F}_{i\pm\frac{1}{2}} \approx F_{i\pm\frac{1}{2}}$: polynomial reconstructions

FVM

- FV formulation

$$\frac{1}{h_i}\left(F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}\right) - \bar{f}_i = 0, i = 1, \ldots, I$$

$F_{i\pm\frac{1}{2}} = v(x_{i\pm\frac{1}{2}})\phi(x_{i\pm\frac{1}{2}}) - \kappa(x_{i\pm\frac{1}{2}})\phi'(x_{i\pm\frac{1}{2}}), \bar{f}_i = \frac{1}{h_i}\int_{K_i} f(\xi)\,\mathrm{d}\xi$

- goal — to compute an approximation to the mean value of ϕ in each cell of the mesh: $\phi_i \approx \frac{1}{h_i}\int_{K_i}\phi\,\mathrm{d}x$
- the approximation to the mean value of f over cell K_i, $f_i \approx \frac{1}{h_i}\int_{K_i} f\,\mathrm{d}x$, will be computed by gaussian quadrature
- the way that the numerical diffusive and convective fluxes are computed characterize the FVM scheme
- how to approximate numerically the fluxes with very-high precision $\mathcal{F}_{i\pm\frac{1}{2}} \approx F_{i\pm\frac{1}{2}}$: polynomial reconstructions

POLYNOMIAL RECONSTRUCTIONS

- conservative reconstruction: where there is an information
  - cells:

$$\frac{1}{h_i}\int_{K_i} \widehat{\phi}_i \, \mathrm{d}x = \phi_i, i = 1 \ldots, I$$

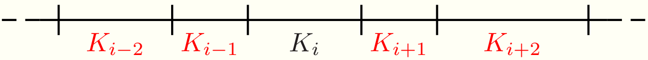
  - Dirichlet outer interface(s):

$$\widehat{\phi}_{\frac{1}{2}}(0) = \phi_{\mathrm{D}}(0) \qquad \widehat{\phi}_{I+\frac{1}{2}}(1) = \phi_{\mathrm{D}}(1)$$

- non-conservative reconstruction: where there is no information
  - inner interfaces:

$$\widetilde{\phi}_{i+\frac{1}{2}}, i = 1 \ldots, I-1$$

$\widehat{S}_i(4)$



- polynomials

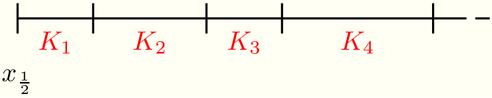
$$\widehat{\phi}_i(x;\mathsf{d}) = \phi_i + \sum_{\alpha=1}^{\mathsf{d}} \widehat{\mathcal{R}}_{i,\alpha} \left[(x - x_i)^\alpha - \frac{1}{h_i} \int_{K_i} (x - c_i)^\alpha \right]$$

- coefficients (determined by the stencils $\widehat{S}_i$): arguments which minimize the functional

$$\widehat{E}_i(\mathcal{R}_i) = \sum_{j \in \widehat{S}_i} \omega_{i,j} \left[\frac{1}{h_j} \int_{K_j} \widehat{\phi}_i(x;\mathsf{d})\,\mathrm{d}x - \phi_j \right]^2$$

Reconstructions for Dirichlet outer interface(s)

$\widetilde{S}_{\frac{1}{2}}(4)$



- polynomial

$$\widehat{\phi}_{\frac{1}{2}}(x;\mathsf{d}) = \phi_{\mathrm{D}}(x_{\frac{1}{2}}) + \sum_{\alpha=1}^{\mathsf{d}} \widehat{\mathcal{R}}_{\frac{1}{2},\alpha}(x - x_{\frac{1}{2}})^{\alpha}$$

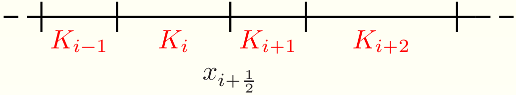
- coefficients (determined by the stencil $\widehat{S}_{\frac{1}{2}}$): arguments which minimize the functional

$$\widehat{E}_{\frac{1}{2}}(\mathcal{R}_{\frac{1}{2}}) = \sum_{j \in S_{\frac{1}{2}}} \omega_{\frac{1}{2},j} \left[\frac{1}{h_j} \int_{K_j} \widehat{\phi}_{\frac{1}{2}}(x;\mathsf{d})\,\mathrm{d}x - \phi_j \right]^2$$

(we proceed in the same way for polynomial $\widehat{\phi}_{I+\frac{1}{2}}$)

RECONSTRUCTIONS FOR INNER INTERFACES

$\widetilde{S}_{i+\frac{1}{2}}(4)$



- polynomials

$$\widetilde{\phi}_{i+\frac{1}{2}}(x;\mathsf{d}) = \sum_{\alpha=0}^{\mathsf{d}} \widetilde{\mathcal{R}}_{i+\frac{1}{2},\alpha}(x - x_{i+\frac{1}{2}})^{\alpha}$$

- coefficients (determined by the stencil $\widetilde{S}_{i+\frac{1}{2}}$): arguments which minimize the functional

$$\widetilde{E}_{i+\frac{1}{2}}(\mathcal{R}_{i+\frac{1}{2}}) = \sum_{j\in S_{i+\frac{1}{2}}} \omega_{i+\frac{1}{2},j} \left[\frac{1}{h_j} \int_{K_j} \widetilde{\phi}_{i+\frac{1}{2}}(x;\mathsf{d})\,\mathrm{d}x - \phi_j \right]^2$$

NUMERICAL FLUXES

$$\mathcal{F}_{i\pm\frac{1}{2}} \approx F_{i\pm\frac{1}{2}} = v(x_{i\pm\frac{1}{2}})\phi(x_{i\pm\frac{1}{2}}) - \kappa(x_{i\pm\frac{1}{2}})\phi'(x_{i\pm\frac{1}{2}}), i = 0\ldots, I$$

- left boundary interface ($i = 0$, D)

$$\mathcal{F}_{\frac{1}{2}}(\Phi) = [v(0)]^{+}\phi_{\mathrm{D}}(0) + [v(0)]^{-}\widehat{\phi}_1(0;\mathsf{d}) - \kappa(0)\widehat{\phi}'_{\frac{1}{2}}(0;\mathsf{d})$$

- left boundary interface ($i = 0$, N)

$$\mathcal{F}_{\frac{1}{2}}(\Phi) = \phi_{\mathrm{T}}(0)$$

- inner interfaces ($i = 1, \ldots, I-1$)

$$\mathcal{F}_{i+\frac{1}{2}}(\Phi) = [v(x_{i+\frac{1}{2}})]^{+}\widehat{\phi}_i(x_{i+\frac{1}{2}};\mathsf{d}) + [v(x_{i+\frac{1}{2}})]^{-}\widehat{\phi}_{i+1}(x_{i+\frac{1}{2}};\mathsf{d}) - \kappa(x_{i+\frac{1}{2}})\widetilde{\phi}'_{i+\frac{1}{2}}(x_{i+\frac{1}{2}};\mathsf{d})$$

- right boundary interface ($i = I$): similar to $i = 0$

RESIDUAL FORM

- based on the linearity of the polynomial reconstructions, the definition of the numerical fluxes, and the finite volume formulation, we obtain an affine operator such that for any $\Phi \in \mathbb{R}^I$, we associate $\mathcal{G}(\Phi) \in \mathbb{R}^I$ given component-wise by

$$\mathcal{G}_i(\Phi) = \frac{1}{h_i} \left(\mathcal{F}_{i+\frac{1}{2}}(\Phi) - \mathcal{F}_{i-\frac{1}{2}}(\Phi) \right) - f_i$$

- the numerical solution is given by vector $\Phi^\dagger = (\phi_i^\dagger)_{i=1,\dots,I}$ which is the solution of the linear problem

$$\mathcal{G}(\Phi^\dagger) = 0_I$$

TIME-DEPENDENT CASE

- time-dependent 1D convection-diffusion equation ($\Omega =]0,1[$, $t_\mathrm{f} \in \mathbb{R}^+$)

$$\partial_t \phi + \partial_x(v\phi) - \partial_x(\kappa \partial_x \phi) = f, \quad \text{in } \Omega \times]0, t_\mathrm{f}[$$

- boundary conditions ($\bar{x}$ is a boundary point):
  - Dirichlet: $\phi(\bar{x}, t) = \phi_\mathrm{D}(\bar{x}, t)$
  - Neumann: $v(\bar{x}, t)\phi(\bar{x}, t) - \kappa(\bar{x}, t)\partial_x \phi(\bar{x}, t) = \phi_\mathrm{T}(\bar{x}, t)$
- initial condition: $\phi(x, 0) = \phi^0(x) \quad \text{in } \bar{\Omega}$
- unknown $\phi : [0,1] \times [0, t_\mathrm{f}] \to \mathbb{R}$
- data (regular)
  - diffusion coefficient $\kappa : [0,1] \times [0, t_\mathrm{f}] \to \mathbb{R}^+$
  - convection coefficient (=velocity) $v : [0,1] \times [0, t_\mathrm{f}] \to \mathbb{R}$
  - source $f : [0,1] \times [0, t_\mathrm{f}] \to \mathbb{R}$
  - boundary conditions $\phi_D(x, t) : \{0, 1\} \times [0, t_\mathrm{f}] \to \mathbb{R}$
  - initial condition $\phi^0 : [0,1] \to \mathbb{R}$

TIME-DEPENDENT CASE

- time-dependent 1D convection-diffusion equation ($\Omega =]0,1[$, $t_\mathrm{f} \in \mathbb{R}^+$)

$$\partial_t \phi + \partial_x(v\phi) - \partial_x(\kappa \partial_x \phi) = f, \quad \text{in } \Omega \times]0, t_\mathrm{f}[$$

- boundary conditions ($\bar{x}$ is a boundary point):
  - Dirichlet: $\phi(\bar{x}, t) = \phi_\mathrm{D}(\bar{x}, t)$
  - Neumann: $v(\bar{x}, t)\phi(\bar{x}, t) - \kappa(\bar{x}, t)\partial_x \phi(\bar{x}, t) = \phi_\mathrm{T}(\bar{x}, t)$
- initial condition: $\phi(x, 0) = \phi^0(x) \quad \text{in } \bar{\Omega}$
- unknown $\phi : [0,1] \times [0, t_\mathrm{f}] \to \mathbb{R}$
- data (regular)
  - diffusion coefficient $\kappa : [0,1] \times [0, t_\mathrm{f}] \to \mathbb{R}^+$
  - convection coefficient (=velocity) $v : [0,1] \times [0, t_\mathrm{f}] \to \mathbb{R}$
  - source $f : [0,1] \times [0, t_\mathrm{f}] \to \mathbb{R}$
  - boundary conditions $\phi_D(x, t) : \{0,1\} \times [0, t_\mathrm{f}] \to \mathbb{R}$
  - initial condition $\phi^0 : [0,1] \to \mathbb{R}$

TIME-DEPENDENT CASE

- time-dependent 1D convection-diffusion equation ($\Omega =]0,1[$, $t_{\mathrm{f}} \in \mathbb{R}^+$)

$$\partial_t \phi + \partial_x(v\phi) - \partial_x(\kappa \partial_x \phi) = f, \quad \text{in } \Omega \times]0, t_{\mathrm{f}}[$$

- boundary conditions ($\bar{x}$ is a boundary point):
  - Dirichlet: $\phi(\bar{x}, t) = \phi_{\mathrm{D}}(\bar{x}, t)$
  - Neumann: $v(\bar{x}, t)\phi(\bar{x}, t) - \kappa(\bar{x}, t)\partial_x \phi(\bar{x}, t) = \phi_{\mathrm{T}}(\bar{x}, t)$
- initial condition: $\phi(x, 0) = \phi^0(x) \quad \text{in } \bar{\Omega}$
- unknown $\phi : [0,1] \times [0, t_{\mathrm{f}}] \to \mathbb{R}$
- data (regular)
  - diffusion coefficient $\kappa : [0,1] \times [0, t_{\mathrm{f}}] \to \mathbb{R}^+$
  - convection coefficient (=velocity) $v : [0,1] \times [0, t_{\mathrm{f}}] \to \mathbb{R}$
  - source $f : [0,1] \times [0, t_{\mathrm{f}}] \to \mathbb{R}$
  - boundary conditions $\phi_D(x, t) : \{0, 1\} \times [0, t_{\mathrm{f}}] \to \mathbb{R}$
  - initial condition $\phi^0 : [0,1] \to \mathbb{R}$

TIME-DEPENDENT CASE

- time-dependent 1D convection-diffusion equation ($\Omega =]0,1[$, $t_{\mathrm{f}} \in \mathbb{R}^+$)

  $$\partial_t \phi + \partial_x(v\phi) - \partial_x(\kappa \partial_x \phi) = f, \quad \text{in } \Omega \times]0, t_{\mathrm{f}}[$$

- boundary conditions ($\bar{x}$ is a boundary point):
  - Dirichlet: $\phi(\bar{x}, t) = \phi_{\mathrm{D}}(\bar{x}, t)$
  - Neumann: $v(\bar{x}, t)\phi(\bar{x}, t) - \kappa(\bar{x}, t)\partial_x \phi(\bar{x}, t) = \phi_{\mathrm{T}}(\bar{x}, t)$
- initial condition: $\phi(x, 0) = \phi^0(x) \quad \text{in } \bar{\Omega}$
- unknown $\phi : [0,1] \times [0, t_{\mathrm{f}}] \to \mathbb{R}$
- data (regular)
  - diffusion coefficient $\kappa : [0,1] \times [0, t_{\mathrm{f}}] \to \mathbb{R}^+$
  - convection coefficient (=velocity) $v : [0,1] \times [0, t_{\mathrm{f}}] \to \mathbb{R}$
  - source $f : [0,1] \times [0, t_{\mathrm{f}}] \to \mathbb{R}$
  - boundary conditions $\phi_D(x, t) : \{0,1\} \times [0, t_{\mathrm{f}}] \to \mathbb{R}$
  - initial condition $\phi^0 : [0,1] \to \mathbb{R}$

TIME-DEPENDENT CASE

- time-dependent 1D convection-diffusion equation ($\Omega =]0, 1[$, $t_\mathrm{f} \in \mathbb{R}^+$)

$$\partial_t \phi + \partial_x (v\phi) - \partial_x (\kappa \partial_x \phi) = f, \quad \text{in } \Omega \times]0, t_\mathrm{f}[$$

- boundary conditions ($\bar{x}$ is a boundary point):
  - Dirichlet: $\phi(\bar{x}, t) = \phi_\mathrm{D}(\bar{x}, t)$
  - Neumann: $v(\bar{x}, t)\phi(\bar{x}, t) - \kappa(\bar{x}, t)\partial_x \phi(\bar{x}, t) = \phi_\mathrm{T}(\bar{x}, t)$
- initial condition: $\phi(x, 0) = \phi^0(x) \quad \text{in } \bar{\Omega}$
- unknown $\phi : [0, 1] \times [0, t_\mathrm{f}] \to \mathbb{R}$
- data (regular)
  - diffusion coefficient $\kappa : [0, 1] \times [0, t_\mathrm{f}] \to \mathbb{R}^+$
  - convection coefficient (=velocity) $v : [0, 1] \times [0, t_\mathrm{f}] \to \mathbb{R}$
  - source $f : [0, 1] \times [0, t_\mathrm{f}] \to \mathbb{R}$
  - boundary conditions $\phi_D(x, t) : \{0, 1\} \times [0, t_\mathrm{f}] \to \mathbb{R}$
  - initial condition $\phi^0 : [0, 1] \to \mathbb{R}$

MOL — SPACE DISCRETIZATION

$$\frac{\mathrm{d}\bar{\phi}_i}{\mathrm{d}t}(t) + \frac{1}{h_i}\Big(F_{i+\frac{1}{2}}(t) - F_{i-\frac{1}{2}}(t)\Big) - \bar{f}_i(t) = 0,\ t \in]0, t_{\mathrm{f}}]$$

$$\bar{\phi}_i(t) = \frac{1}{h_i}\int_{K_i} \phi(\xi, t)\,\mathrm{d}\xi$$

$$F_{i\pm\frac{1}{2}}(t) = v(x_{i\pm\frac{1}{2}}, t)\phi(x_{i\pm\frac{1}{2}}, t) - \kappa(x_{i\pm\frac{1}{2}}, t)\partial_x\phi(x_{i\pm\frac{1}{2}}, t)$$

$$\bar{f}_i(t) = \frac{1}{h_i}\int_{K_i} f(\xi, t)\,\mathrm{d}\xi$$

$$\frac{\mathrm{d}\phi_i}{\mathrm{d}t}(t) + \underbrace{\frac{1}{h_i}\Big(\mathcal{F}_{i+\frac{1}{2}}(t) - \mathcal{F}_{i-\frac{1}{2}}(t)\Big) - f_i(t)}_{\mathcal{G}_i(t,\Phi(t))} = 0, t \in (0, t_{\mathrm{f}}], i = 1, \dots, I$$

$$\Phi(t) = (\phi_i(t))_{i=1,\dots,I}$$

$$\mathcal{F}_{i+\frac{1}{2}}(t) = \dots,\ i = 0, \dots, I$$

$f_i(t)$ is a gaussian quadrature approximation in space of $\bar{f}_i(t)$

MOL — SPACE DISCRETIZATION

the time parameterized function

$$\Phi^\dagger(t) = (\phi_i^\dagger(t))_{i=1,\ldots,I}$$

is the solution of the differential system

$$\frac{\mathrm{d}\phi_i}{\mathrm{d}t}(t) + \mathcal{G}_i(t, \Phi(t)) = 0, i = 1, \ldots, I$$

where

$$\mathcal{G}_i(t, \Phi(t)) = \frac{1}{h_i}\left(\mathcal{F}_{i+\frac{1}{2}}(t, \Phi(t)) - \mathcal{F}_{i-\frac{1}{2}}(t, \Phi(t))\right) - f_i(t)$$

with the initial conditions

$$\phi_i^\dagger(0) = \bar{\phi}_i^0 \equiv \frac{1}{h_i}\int_{K_i} \phi^0(\xi)\,\mathrm{d}\xi$$

TIME DISCRETIZATION

- $(t^n)_{n=0,\dots,N}$ time discretisation of $[0, t_\mathrm{f} \equiv t^N]$, with

  $t^{n+1} = t^n + \delta^{n+\frac{1}{2}}$

- goal — to compute an approximation to the mean value of ϕ in each cell of the mesh at each time t^n (represented by ϕ_i^n), *i.e.*,

  $$\phi_i^n \approx \frac{1}{h_i} \int_{K_i} \phi(x, t_n)\, \mathrm{d}x, i = 1, \dots, I, n = 0, \dots, N$$

- Φ^n — the vector of unknowns at time t^n, i.e.,

  $$\Phi^n = (\phi_1^n, \dots, \phi_I^n)^T \in \mathbb{R}^I$$

Runge-Kutta methods

Butcher Tableau for an s-stage Runge-Kutta method

$$
\begin{array}{c|ccc}
c_1 & a_{11} & \cdots & a_{1s} \\
\vdots & \vdots & \ddots & \vdots \\
c_s & a_{s1} & \cdots & a_{ss} \\
\hline
 & b_1 & \cdots & b_s
\end{array}
$$

$$t^{n,k} = t^n + \Delta t c_k$$

$$\Phi^{n,k} - \Phi^n + \Delta t \sum_{\ell=1}^{s} a_{k\ell} \mathcal{G}(t^{n,\ell}, \Phi^{n,\ell}) = 0_I, \quad k = 1, \ldots, s$$

$$\Phi^{n+1} = \Phi^n - \Delta t \sum_{k=1}^{s} b_k \mathcal{G}(t^{n,k}, \Phi^{n,k})$$

(classical) RK3

Butcher Tableau for the classical 3-stage RK3 method

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 1 & -1 & 2 & 0 \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}$$

D+D	I	t^2		$x(x-1)t^2$		$\cosh(x)\exp(-t)$	
		err	ord	err	ord	err	ord
		with Butcher Tableau					
$\mathbb{P}_5(6)$ $\Delta t = \frac{1}{3}h^2$	10	1.8E−06	—	8.1E−09	—	1.1E−06	—
	20	1.1E−07	4.0	1.3E−10	6.0	6.8E−08	4.0
	30	2.2E−08	4.0	1.1E−11	6.0	1.3E−08	4.0

(CLASSICAL) RK3

$\kappa = 1, v = 0, \phi(x,t) = t^2, \mathrm{D+D}$

$$\Phi^0 = (0, \ldots, 0)^T$$

$$\Phi^{0,1} = (0, \ldots, 0)^T$$

$$\Phi^{0,2} = (0, \ldots, 0)^T$$

$$\Phi^{0,3} = \left(2\Delta t^2 + \frac{\Delta t^3}{h^2}, 2\Delta t^2, \ldots, 2\Delta t^2, 2\Delta t^2 + \frac{\Delta t^3}{h^2}\right)^T$$

$$\Phi^1 = \Delta t^2 \left(1, 1, 1, \ldots, 1, 1, 1\right)^T + \left(-\frac{\Delta t^4}{2h^4}, \frac{\Delta t^4}{6h^4}, 0, \ldots, 0, \frac{\Delta t^4}{6h^4}, -\frac{\Delta t^4}{2h^4}\right)^T$$

Extended Butcher Tableau (D+D)

- to overcome the incompatibility problem, we shall consider a relaxation of the discretization considering now that the time discretizations for the source term and for the Dirichlet condition can be different
- let

$$\Phi_{\mathrm{D}}^{n,k} = \begin{pmatrix} \phi_{\mathrm{D}}(x_{\mathrm{L}}, t^{n,k}) \\ \phi_{\mathrm{D}}(x_{\mathrm{R}}, t^{n,k}) \end{pmatrix}$$

- we re-qualify the residual operator setting

$$\mathcal{G}^{n,k} = \mathcal{G}(t^{n,k}, \Phi^{n,k}, F^{n,k}, \Phi_{\mathrm{D}\star}^{n,k}), \quad \Phi_{\mathrm{D}\star}^{n,k} = \sum_{\ell=1}^{s} p_{k,\ell} \Phi_{\mathrm{D}}^{n,\ell}, \; k = 1, \dots, s$$

- **Principle:** The time discretizations of the source term and the Dirichlet condition are compatible up to degree d if the scheme exactly solves the solutions t^m, $m = 0, \dots, d$, constant in space

Extended Butcher Tableau (D+D)

- to overcome the incompatibility problem, we shall consider a relaxation of the discretization considering now that the time discretizations for the source term and for the Dirichlet condition can be different
- let

$$\Phi_{\mathrm{D}}^{n,k} = \begin{pmatrix} \phi_{\mathrm{D}}(x_{\mathrm{L}}, t^{n,k}) \\ \phi_{\mathrm{D}}(x_{\mathrm{R}}, t^{n,k}) \end{pmatrix}$$

- we re-qualify the residual operator setting

$$\mathcal{G}^{n,k} = \mathcal{G}(t^{n,k}, \Phi^{n,k}, F^{n,k}, \Phi_{\mathrm{D}\star}^{n,k}), \ \Phi_{\mathrm{D}\star}^{n,k} = \sum_{\ell=1}^{s} p_{k,\ell} \Phi_{\mathrm{D}}^{n,\ell}, \ k = 1, \dots, s$$

- **Principle:** The time discretizations of the source term and the Dirichlet condition are compatible up to degree d if the scheme exactly solves the solutions t^m, $m = 0, \dots, d$, constant in space

Extended Butcher Tableau (D+D)

- to overcome the incompatibility problem, we shall consider a relaxation of the discretization considering now that the time discretizations for the source term and for the Dirichlet condition can be different
- let

$$\Phi_{\mathrm{D}}^{n,k} = \begin{pmatrix} \phi_{\mathrm{D}}(x_{\mathrm{L}}, t^{n,k}) \\ \phi_{\mathrm{D}}(x_{\mathrm{R}}, t^{n,k}) \end{pmatrix}$$

- we re-qualify the residual operator setting

$$\mathcal{G}^{n,k} = \mathcal{G}(t^{n,k}, \Phi^{n,k}, F^{n,k}, \Phi_{\mathrm{D}\star}^{n,k}), \quad \Phi_{\mathrm{D}\star}^{n,k} = \sum_{\ell=1}^{s} p_{k,\ell} \Phi_{\mathrm{D}}^{n,\ell}, \; k = 1, \ldots, s$$

- **Principle:** The time discretizations of the source term and the Dirichlet condition are compatible up to degree d if the scheme exactly solves the solutions t^m, $m = 0, \ldots, d$, constant in space

Extended Butcher Tableau (D+D)

- to overcome the incompatibility problem, we shall consider a relaxation of the discretization considering now that the time discretizations for the source term and for the Dirichlet condition can be different
- let

$$\Phi_{\mathrm{D}}^{n,k} = \begin{pmatrix} \phi_{\mathrm{D}}(x_{\mathrm{L}}, t^{n,k}) \\ \phi_{\mathrm{D}}(x_{\mathrm{R}}, t^{n,k}) \end{pmatrix}$$

- we re-qualify the residual operator setting

$$\mathcal{G}^{n,k} = \mathcal{G}(t^{n,k}, \Phi^{n,k}, F^{n,k}, \Phi_{\mathrm{D}\star}^{n,k}), \quad \Phi_{\mathrm{D}\star}^{n,k} = \sum_{\ell=1}^{s} p_{k,\ell} \Phi_{\mathrm{D}}^{n,\ell}, \ k = 1, \ldots, s$$

- **Principle:** The time discretizations of the source term and the Dirichlet condition are compatible up to degree d if the scheme exactly solves the solutions t^m, $m = 0, \ldots, d$, constant in space

Extended Butcher Tableau (D+D)

- application of the **Principle** with $\kappa = 1$, $v = 0$

$$Q^d p^T = \widehat{Q}^d a^T + E_1^{d+1,s} \qquad \Phi_{\mathrm{D}\star}^{n,k} = \sum_{\ell=1}^{s} p_{k,\ell} \Phi_{\mathrm{D}}^{n,\ell}$$

$$Q^d = \underbrace{\begin{pmatrix} (c_1)^0 & \cdots & (c_s)^0 \\ (c_1)^1 & \cdots & (c_s)^1 \\ \vdots & \ddots & \vdots \\ (c_1)^d & \cdots & (c_s)^d \end{pmatrix}}_{(d+1)\times s} \quad \widehat{Q}^d = \underbrace{\begin{pmatrix} 0 & \cdots & 0 \\ 1(c_1)^0 & \cdots & 1(c_s)^0 \\ \vdots & \ddots & \vdots \\ d(c_1)^{d-1} & \cdots & d(c_s)^{d-1} \end{pmatrix}}_{(d+1)\times s} \quad E_1^{d+1,s} = \underbrace{\begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}}_{(d+1)\times 1}$$

- for the classical RK3, all coefficients c_ℓ are different
- for the classical RK3, $s = d + 1$, that is, the Vandermonde matrix Q^d is square and invertible, which implies the existence and uniqueness of matrix p

(MODIFIED) RK3

Extended Butcher Tableau for the classical 3-stage RK3 method

$$
\begin{array}{c|ccc|ccc}
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & 0 & 0 & -\frac{1}{2} & 2 & -\frac{1}{2} \\
1 & -1 & 2 & 0 & 2 & -4 & 3 \\
\hline
 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & & &
\end{array}
$$

D+D	I	t^2 err	t^2 ord	$x(x-1)t^2$ err	$x(x-1)t^2$ ord	$\cosh(x)\exp(-t)$ err	$\cosh(x)\exp(-t)$ ord
with Butcher Tableau							
$\mathbb{P}_5(6)$, $\Delta t = \frac{1}{3}h^2$	10	1.8E−06	—	8.1E−09	—	1.1E−06	—
	20	1.1E−07	4.0	1.3E−10	6.0	6.8E−08	4.0
	30	2.2E−08	4.0	1.1E−11	6.0	1.3E−08	4.0
with Extended Butcher Tableau							
$\mathbb{P}_5(6)$, $\Delta t = \frac{1}{3}h^2$	10	4.2E−17	—	8.1E−09	—	7.3E−08	NA
	20	1.0E−16	—	1.3E−10	6.0	1.3E−09	5.9
	30	2.2E−16	—	1.1E−11	6.0	1.1E−10	5.9

RK4

0	0	0	0	0	1	0	0	0	0
$\frac{1}{2}$	$\frac{1}{2}$	0	0	0	$-\frac{7}{6}$	6	$-\frac{16}{3}$	$\frac{3}{2}$	$\frac{1}{2}$
$\frac{1}{2}$	0	$\frac{1}{2}$	0	0	$\frac{5}{6}$	-2	$\frac{8}{3}$	$-\frac{1}{2}$	$\frac{3}{4}$
1	0	0	1	0	$\frac{2}{3}$	-4	$\frac{16}{3}$	-1	1
	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{6}$					

- since $c_2 = c_3$, we can not directly apply the methodology developed in the previous section because matrix Q^4 is singular
- to overcome the problem, we introduce a new vector $z = (z_1, z_2, z_3, z_4)^T$ and new time stages $\tau^{n,k} = t^n + z_k \Delta t$, $k = 1, \ldots, s$
- we choose $z = (0, \frac{1}{2}, \frac{3}{4}, 1)$
- for the classical RK4, $s = d + 1$, that is, the Vandermonde matrix Q^d is square and now, with the new vector z, is also invertible, which implies the existence and uniqueness of matrix p

RK4

0	0	0	0	0	1	0	0	0	0
$\frac{1}{2}$	$\frac{1}{2}$	0	0	0	$-\frac{7}{6}$	6	$-\frac{16}{3}$	$\frac{3}{2}$	$\frac{1}{2}$
$\frac{1}{2}$	0	$\frac{1}{2}$	0	0	$\frac{5}{6}$	-2	$\frac{8}{3}$	$-\frac{1}{2}$	$\frac{3}{4}$
1	0	0	1	0	$\frac{2}{3}$	-4	$\frac{16}{3}$	-1	1
	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{6}$					

- since $c_2 = c_3$, we can not directly apply the methodology developed in the previous section because matrix Q^4 is singular
- to overcome the problem, we introduce a new vector $z = (z_1, z_2, z_3, z_4)^T$ and new time stages $\tau^{n,k} = t^n + z_k \Delta t$, $k = 1, \ldots, s$
- we choose $z = (0, \frac{1}{2}, \frac{3}{4}, 1)$
- for the classical RK4, $s = d + 1$, that is, the Vandermonde matrix Q^d is square and now, with the new vector z, is also invertible, which implies the existence and uniqueness of matrix p

RK4

0	0	0	0	0	1	0	0	0	0
$\frac{1}{2}$	$\frac{1}{2}$	0	0	0	$-\frac{7}{6}$	6	$-\frac{16}{3}$	$\frac{3}{2}$	$\frac{1}{2}$
$\frac{1}{2}$	0	$\frac{1}{2}$	0	0	$\frac{5}{6}$	-2	$\frac{8}{3}$	$-\frac{1}{2}$	$\frac{3}{4}$
1	0	0	1	0	$\frac{2}{3}$	-4	$\frac{16}{3}$	-1	1
	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{6}$					

- since $c_2 = c_3$, we can not directly apply the methodology developed in the previous section because matrix Q^4 is singular
- to overcome the problem, we introduce a new vector $z = (z_1, z_2, z_3, z_4)^T$ and new time stages $\tau^{n,k} = t^n + z_k \Delta t$, $k = 1, \ldots, s$
- we choose $z = (0, \frac{1}{2}, \frac{3}{4}, 1)$
- for the classical RK4, $s = d + 1$, that is, the Vandermonde matrix Q^d is square and now, with the new vector z, is also invertible, which implies the existence and uniqueness of matrix p

RK4

$$
\begin{array}{c|cccc|cccc|c}
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & -\frac{7}{6} & 6 & -\frac{16}{3} & \frac{3}{2} & \frac{1}{2} \\
\frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 & \frac{5}{6} & -2 & \frac{8}{3} & -\frac{1}{2} & \frac{3}{4} \\
1 & 0 & 0 & 1 & 0 & \frac{2}{3} & -4 & \frac{16}{3} & -1 & 1 \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} & & & & &
\end{array}
$$

- since $c_2 = c_3$, we can not directly apply the methodology developed in the previous section because matrix Q^4 is singular
- to overcome the problem, we introduce a new vector $z = (z_1, z_2, z_3, z_4)^T$ and new time stages $\tau^{n,k} = t^n + z_k \Delta t$, $k = 1, \dots, s$
- we choose $z = (0, \frac{1}{2}, \frac{3}{4}, 1)$
- for the classical RK4, $s = d + 1$, that is, the Vandermonde matrix Q^d is square and now, with the new vector z, is also invertible, which implies the existence and uniqueness of matrix p

RK4

$$
\begin{array}{c|cccc|cccc|c}
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & -\frac{7}{6} & 6 & -\frac{16}{3} & \frac{3}{2} & \frac{1}{2} \\
\frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 & \frac{5}{6} & -2 & \frac{8}{3} & -\frac{1}{2} & \frac{3}{4} \\
1 & 0 & 0 & 1 & 0 & \frac{2}{3} & -4 & \frac{16}{3} & -1 & 1 \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} & & & & &
\end{array}
$$

- since $c_2 = c_3$, we can not directly apply the methodology developed in the previous section because matrix Q^4 is singular
- to overcome the problem, we introduce a new vector $z = (z_1, z_2, z_3, z_4)^T$ and new time stages $\tau^{n,k} = t^n + z_k \Delta t$, $k = 1, \ldots, s$
- we choose $z = (0, \frac{1}{2}, \frac{3}{4}, 1)$
- for the classical RK4, $s = d + 1$, that is, the Vandermonde matrix Q^d is square and now, with the new vector z, is also invertible, which implies the existence and uniqueness of matrix p

RK4

$$
\begin{array}{c|cccc|cccc|c}
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & -\frac{7}{6} & 6 & -\frac{16}{3} & \frac{3}{2} & \frac{1}{2} \\
\frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 & \frac{5}{6} & -2 & \frac{8}{3} & -\frac{1}{2} & \frac{3}{4} \\
1 & 0 & 0 & 1 & 0 & \frac{2}{3} & -4 & \frac{16}{3} & -1 & 1 \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} & & & & &
\end{array}
$$

- since $c_2 = c_3$, we can not directly apply the methodology developed in the previous section because matrix Q^4 is singular
- to overcome the problem, we introduce a new vector $z = (z_1, z_2, z_3, z_4)^T$ and new time stages $\tau^{n,k} = t^n + z_k \Delta t$, $k = 1, \ldots, s$
- we choose $z = (0, \frac{1}{2}, \frac{3}{4}, 1)$
- for the classical RK4, $s = d + 1$, that is, the Vandermonde matrix Q^d is square and now, with the new vector z, is also invertible, which implies the existence and uniqueness of matrix p

RK4

D+D, $\kappa = 1$, $v = 0$, $\phi(x,t) = \cosh(x)\exp(-t)$					
	I	BT		EBT	
		E_∞	O_∞	E_∞	O_∞
	10	2.8E−06	—	3.5E−09	—
$\mathbb{P}_7(8)$	20	1.6E−07	4.1	5.2E−11	6.1
$\Delta t = \frac{1}{3}h^2$	40	1.0E−08	4.0	8.2E−13	6.0
	80	6.4E−10	4.0	1.1E−14	6.3

ESDIRK4

- if $a_{i,j} = 0$ for $i < j$ and $a_{1,1} = 0$ with all diagonal entries equal, we have an explicit singly diagonally implicit Runge-Kutta — ESDIRK
- if $s > d + 1$ corresponds to an under-determined linear system associated to a maximal rank matrix Q^d — one has to develop a strategy to determine a unique matrix p. We here propose two ways to determine matrix p namely:
  - LS-way: find p in the Least Square sense
  - AC-way: Augment the number of Constraints adding polynomial functions t^{d+1}, …, t^{s-1} such that we get a invertible Vandermonde square matrix Q^{s-1}

$$
\begin{array}{c|cccccc|cccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -\frac{738}{2093} & -\frac{193}{9366} & -\frac{151}{1016} & -\frac{490}{1663} & 0 \\
\frac{1}{2} & \frac{1}{4} & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{83}{250} & \frac{8611}{62500} & -\frac{1743}{31250} & \frac{1}{4} & 0 & 0 & 0 & 0 & \frac{895}{618} & \frac{1654}{1551} & \frac{501}{1046} & \frac{1703}{2211} & 0 \\
\frac{31}{50} & \frac{5012029}{34652500} & -\frac{654441}{2922500} & \frac{174375}{388108} & \frac{1}{4} & 0 & 0 & 0 & -\frac{455}{1506} & -\frac{319}{5103} & \frac{922}{1679} & -\frac{805}{4378} & 0 \\
\frac{17}{20} & \frac{15267082809}{155376265600} & -\frac{71443401}{120774400} & \frac{730878875}{902184768} & \frac{2285395}{8070912} & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & \frac{82889}{524892} & 0 & \frac{15625}{83664} & \frac{69875}{102672} & -\frac{2260}{8211} & \frac{1}{4} & 0 & \frac{165}{799} & \frac{303}{18133} & \frac{400}{3319} & \frac{573}{809} & 1 \\
\hline
 & \frac{82889}{524892} & 0 & \frac{15625}{83664} & \frac{69875}{102672} & -\frac{2260}{8211} & \frac{1}{4} & & & & & &
\end{array}
$$

ESDIRK4

- if $a_{i,j} = 0$ for $i < j$ and $a_{1,1} = 0$ with all diagonal entries equal, we have an explicit singly diagonally implicit Runge-Kutta — ESDIRK
- if $s > d + 1$ corresponds to an under-determined linear system associated to a maximal rank matrix Q^d — one has to develop a strategy to determine a unique matrix p. We here propose two ways to determine matrix p namely:
  - LS-way: find p in the Least Square sense
  - AC-way: Augment the number of Constraints adding polynomial functions t^{d+1}, ..., t^{s-1} such that we get a invertible Vandermonde square matrix Q^{s-1}

$$
\begin{array}{c|cccccc|cccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -\frac{738}{2093} & -\frac{193}{9366} & -\frac{151}{1016} & -\frac{490}{1663} & 0 \\
\frac{1}{2} & \frac{1}{4} & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{83}{250} & \frac{8611}{62500} & -\frac{1743}{31250} & \frac{1}{4} & 0 & 0 & 0 & 0 & \frac{895}{618} & \frac{1654}{1551} & \frac{501}{1046} & \frac{1703}{2211} & 0 \\
\frac{31}{50} & \frac{5012029}{34652500} & -\frac{654441}{2922500} & \frac{174375}{388108} & \frac{1}{4} & 0 & 0 & 0 & -\frac{455}{1506} & -\frac{319}{5103} & \frac{922}{1679} & -\frac{805}{4378} & 0 \\
\frac{17}{20} & \frac{15267082809}{155376265600} & -\frac{71443401}{120774400} & \frac{730878875}{902184768} & \frac{2285395}{8070912} & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & \frac{82889}{524892} & 0 & \frac{15625}{83664} & \frac{69875}{102672} & -\frac{2260}{8211} & \frac{1}{4} & 0 & \frac{165}{799} & \frac{303}{18133} & \frac{400}{3319} & \frac{573}{809} & 1 \\
\hline
 & \frac{82889}{524892} & 0 & \frac{15625}{83664} & \frac{69875}{102672} & -\frac{2260}{8211} & \frac{1}{4} & & & & & &
\end{array}
$$

ESDIRK4

- if $a_{i,j} = 0$ for $i < j$ and $a_{1,1} = 0$ with all diagonal entries equal, we have an explicit singly diagonally implicit Runge-Kutta — ESDIRK
- if $s > d + 1$ corresponds to an under-determined linear system associated to a maximal rank matrix Q^d — one has to develop a strategy to determine a unique matrix p. We here propose two ways to determine matrix p namely:
  - LS-way: find p in the Least Square sense
  - AC-way: Augment the number of Constraints adding polynomial functions t^{d+1}, …, t^{s-1} such that we get a invertible Vandermonde square matrix Q^{s-1}

$$
\begin{array}{c|cccccc|cccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -\frac{738}{2093} & -\frac{193}{9366} & -\frac{151}{1016} & -\frac{490}{1663} & 0 \\
\frac{1}{2} & \frac{1}{4} & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{83}{250} & \frac{8611}{62500} & -\frac{1743}{31250} & \frac{1}{4} & 0 & 0 & 0 & 0 & \frac{895}{618} & \frac{1654}{1551} & \frac{501}{1046} & \frac{1703}{2211} & 0 \\
\frac{31}{50} & \frac{5012029}{34652500} & -\frac{654441}{2922500} & \frac{174375}{388108} & \frac{1}{4} & 0 & 0 & 0 & -\frac{455}{1506} & -\frac{319}{5103} & \frac{922}{1679} & -\frac{805}{4378} & 0 \\
\frac{17}{20} & \frac{15267082809}{155376265600} & -\frac{71443401}{120774400} & \frac{730878875}{902184768} & \frac{2285395}{8070912} & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & \frac{82889}{524892} & 0 & \frac{15625}{83664} & \frac{69875}{102672} & -\frac{2260}{8211} & \frac{1}{4} & 0 & \frac{165}{799} & \frac{303}{18133} & \frac{400}{3319} & \frac{573}{809} & 1 \\
\hline
 & \frac{82889}{524892} & 0 & \frac{15625}{83664} & \frac{69875}{102672} & -\frac{2260}{8211} & \frac{1}{4} & & & & & &
\end{array}
$$

ESDIRK4

- if $a_{i,j} = 0$ for $i < j$ and $a_{1,1} = 0$ with all diagonal entries equal, we have an explicit singly diagonally implicit Runge-Kutta — ESDIRK
- if $s > d + 1$ corresponds to an under-determined linear system associated to a maximal rank matrix Q^d — one has to develop a strategy to determine a unique matrix p. We here propose two ways to determine matrix p namely:
  - LS-way: find p in the Least Square sense
  - AC-way: Augment the number of Constraints adding polynomial functions t^{d+1}, …, t^{s-1} such that we get a invertible Vandermonde square matrix Q^{s-1}

$$
\begin{array}{c|cccccc|cccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -\frac{738}{2093} & -\frac{193}{9366} & -\frac{151}{1016} & -\frac{490}{1663} & 0 \\
\frac{1}{2} & \frac{1}{4} & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{83}{250} & \frac{8611}{62500} & -\frac{1743}{31250} & \frac{1}{4} & 0 & 0 & 0 & 0 & \frac{895}{618} & \frac{1654}{1551} & \frac{501}{1046} & \frac{1703}{2211} & 0 \\
\frac{31}{50} & \frac{5012029}{34652500} & -\frac{654441}{2922500} & \frac{174375}{388108} & \frac{1}{4} & 0 & 0 & 0 & -\frac{455}{1506} & -\frac{319}{5103} & \frac{922}{1679} & -\frac{805}{4378} & 0 \\
\frac{17}{20} & \frac{15267082809}{155376265600} & -\frac{71443401}{120774400} & \frac{730878875}{902184768} & \frac{2285395}{8070912} & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & \frac{82889}{524892} & 0 & \frac{15625}{83664} & \frac{69875}{102672} & -\frac{2260}{8211} & \frac{1}{4} & 0 & \frac{165}{799} & \frac{303}{18133} & \frac{400}{3319} & \frac{573}{809} & 1 \\
\hline
 & \frac{82889}{524892} & 0 & \frac{15625}{83664} & \frac{69875}{102672} & -\frac{2260}{8211} & \frac{1}{4} & & & & & &
\end{array}
$$

ESDIRK4

D+D, $\kappa = 1$, $v = 0$, $\phi(x,t) = \cosh(x)\exp(-t)$							
	I	BT		EBT (LS-way)		EBT (AC-way)	
		E_∞	O_∞	E_∞	O_∞	E_∞	O_∞
$\mathbb{P}_3(4)$ $\Delta t = 10h$	20	1.3E−04	—	2.0E−05	—	2.2E−05	—
	40	1.1E−05	3.6	1.1E−06	4.2	1.1E−06	4.3
	80	1.2E−06	3.2	6.6E−08	4.0	6.7E−08	4.1
	160	1.3E−07	3.1	4.2E−09	4.0	4.0E−09	4.1
$\mathbb{P}_5(6)$ $\Delta t = h^{1.5}$	10	4.3E−08	—	3.6E−08	—	3.5E−08	—
	20	1.1E−09	5.4	6.0E−10	5.9	5.9E−10	5.9
	40	3.4E−11	4.9	9.8E−12	5.9	9.7E−12	5.9
	80	1.4E−12	4.6	2.0E−13	5.6	2.0E−13	5.6

Neumann boundary conditions

- the principle proposed in the Dirichlet case can not be here applied since a constant in space function gives rise to homogeneous Neumann conditions
- therefore, we introduce a slightly different generic principle to derive the two discretizations:
- **Principle:** The time discretizations of the source term and the Neumann conditions are compatible up to degree d if the scheme exactly solves the solutions xt^m, $m = 0, \ldots, d$, linear in space
- it can be deduced that we can use the same time discretization both for the Dirichlet and the Neumann conditions characterized by the same *Extended Butcher Tableau*.

Neumann boundary conditions + RK3

N+N, $\kappa = 1$, $v = 0$, $\phi(x,t) = \cosh(x)\exp(-t)$					
	I	BT		EBT	
		E_∞	O_∞	E_∞	O_∞
$\mathbb{P}_7(8)$ $\Delta t = \frac{1}{3}h^2$	10	7.1E−09	—	3.5E−10	—
	14	1.3E−09	5.0	3.1E−11	7.2
	17	5.1E−10	5.0	8.1E−12	6.9
	20	2.3E−10	5.0	2.9E−12	6.3

FINAL REMARKS

- we have presented a finite volume method which provides very high-order approximations for regular time-dependent case convection-diffusion problem in 1D both with Dirichlet and Neumann boundary conditions
- we are working in the generalization in order to consider multi-step methods, namely methods like Adams-Bashforth and Adams-Moulton
- the same orders of convergence were already obtained for the 2D and 3D steady-state convection-diffusion problems, so we want to test the developed methodology for the 2D and 3D time-dependent convection-diffusion problems

FINAL REMARKS

- we have presented a finite volume method which provides very high-order approximations for regular time-dependent case convection-diffusion problem in 1D both with Dirichlet and Neumann boundary conditions
- we are working in the generalization in order to consider multi-step methods, namely methods like Adams-Bashforth and Adams-Moulton
- the same orders of convergence were already obtained for the 2D and 3D steady-state convection-diffusion problems, so we want to test the developed methodology for the 2D and 3D time-dependent convection-diffusion problems

FINAL REMARKS

- we have presented a finite volume method which provides very high-order approximations for regular time-dependent case convection-diffusion problem in 1D both with Dirichlet and Neumann boundary conditions
- we are working in the generalization in order to consider multi-step methods, namely methods like Adams-Bashforth and Adams-Moulton
- the same orders of convergence were already obtained for the 2D and 3D steady-state convection-diffusion problems, so we want to test the developed methodology for the 2D and 3D time-dependent convection-diffusion problems