

# The Structural Method

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- 2 Structural method for 1D (space discretization)
- 3 Structural method for ODE (time discretization)
- 4 One dimensional non-stationary equations

# From compact schemes to structural schemes

# Physical equations vs Structural equations

Consider the simple one-dimensional C-D-R equations

$$-\kappa\phi'' + u\phi' + r\phi = f, \quad \text{on } [0, 1]$$

with Robin condition

$$\alpha(x)\phi'(x) + \beta(x)\phi(x) = g(x), \quad x = 0, 1.$$

Grid  $x_i = i\Delta x$ ,  $i = 0, \dots, I$ . A popular centered FD scheme reads

$$-\kappa \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} + u \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} + r\phi_i = f_i$$

with  $\phi_i \approx \phi(x_i)$ .

# Physical equations vs Structural equations

Rewrite with  $Z_i \approx \phi(x_i)$ ,  $D_i \approx \phi'(x_i)$ ,  $S_i \approx \phi''(x_i)$ .

$$-\kappa S_i + uD_i + rZ_i = f_i, \quad (\text{1st Physical Equation})$$

with Robin condition (2nd Physical Equation)

$$\alpha_N(0)D_0 + \alpha_D(0)Z_0 = g(0),$$

$$\alpha_N(1)D_I + \alpha_D(1)Z_I = g(1),$$

and

$$S_i = \frac{Z_{i+1} - 2Z_i + Z_{i-1}}{\Delta x^2}, \quad (\text{1st Structural Equation})$$

$$D_i = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}, \quad (\text{2nd Structural Equation}).$$

☞ PE only deals with physics, SE only deals with mesh structure.

# Implicit and explicit Structural equations

- ☞ Change of scheme  $\Leftrightarrow$  change the SEs (PEs are the same).
- ☞ Use implicit SE  $\Rightarrow$  some classical compact schemes (HOC).

**Hermitian compact scheme** (Orzar & Israeli 1974, Adam 1975, )

$$\begin{aligned}\phi(x_{i+1}) - \phi(x_{i-1}) &= \int_{x_{i-1}}^{x_{i+1}} \phi'(s) ds \Rightarrow \\ Z_{i+1} - Z_{i-1} &= \frac{\Delta x}{6} (D_{i-1} + 4D_i + D_{i+1}). \quad (SE1)\end{aligned}$$

$$\begin{aligned}\frac{\phi(x_{i+1}) + \phi(x_{i-1}) - 2\phi(x_i)}{\Delta x^2} &= \phi''(x_i) + \frac{\Delta x^2}{12} \phi^{(4)}(x_i) + O(\Delta x^4) \\ \frac{\phi''(x_{i+1}) + \phi''(x_{i-1}) - 2\phi''(x_i)}{\Delta x^2} &= \phi^{(4)}(x_i) + O(\Delta x^2) \Rightarrow \\ \frac{Z_{i+1} + Z_{i-1} - 2Z_i}{\Delta x^2} &= \frac{S_{i-1} + 10S_i + S_{i+1}}{12}. \quad (SE2)\end{aligned}$$

## More on Hermitian scheme

- ☞ Philosophy (70s-90s): we see  $D$  or  $S$  as functions of  $Z$  to produce an implicit scheme with respect to  $Z$ .
- ☞ A lot of variants to increase the order and improve the spectral resolution (Kreiss & al. 1986, Lele 1992).

Typically the Hermitian schemes read

$$\sum_{k=-2}^2 a_k Z_{i+k} = \sum_{k=-2}^2 b_k D_{i+k}, \quad (SE1)$$

$$\sum_{k=-2}^2 c_k Z_{i+k} = \sum_{k=-2}^2 d_k S_{i+k}. \quad (SE2)$$

Together with (PE1), we have 3 Equations and 3 Unknowns by node (let's forget the BCs for the moment).

We have a configuration (PE1)-(SE1)-(SE2)

# The Combined Compact Difference scheme

☞ Chu and Fan 1997, 1998 introduce two major ideas:

- 1 don't see  $D$  and  $S$  as function of  $Z$  but as **real Unknowns** of the problem (with the same status as  $Z$ );
- 2 a Structural Equation is a combination of  $Z$ ,  $D$  and  $S$  over a small stencil.

SE equations take the form

$$\sum_{k=-1}^1 a_k Z_{i+k} + \sum_{k=-1}^1 b_k D_{i+k} + \sum_{k=-1}^1 c_k S_{i+k} = 0.$$

Coefficients are determined using Taylor expansions and we eliminate the maximum number of terms.

- ☞ C & F produce 2 structural equations leading to a 6th order compact scheme.
- ☞ Excellent spectral resolution. No dissipation, very few dispersion.
- ☞ Since the 2000s', a lot of variations (non-uniform, larger stencil, system,...)



# Structural method philosophy

- 1 Each node (or cell) contains several information:  $Z_i, D_i, S_i$ .
- 2 Physical Equations are local (no coupling between nodes).
- 3 Structural Equations linearly connect information of the neighbour nodes independently of the physics.
- 4 We need the same number of equations than the number of unknowns: mixe PEs and SEs.
- 5 Build families of SE (Hermitian and CCD are particular cases).
- 6 Not necessarily on the base of accuracy (stability, positivity, spectral resolution).
- 7 The choice of PEs and SEs may be different form one node to another one (BCs treatment).

# The structural method for 1D problem

- $\Omega = ]0, 1[$  with grid  $x_0 = 0, x_i, x_I = 1$ .
- We introduce a functional to design three-points 9-coefs SEs.

$$\begin{aligned}\mathcal{E}_i(\mathbf{a}; \phi) &= \sum_{k=-1}^{k=1} a_{i,k}^{(0)} \phi^{(0)}(x_{i+k}) \\ &+ \sum_{k=-1}^{k=1} a_{i,k}^{(1)} \phi^{(1)}(x_{i+k}) \\ &+ \sum_{k=-1}^{k=1} a_{i,k}^{(2)} \phi^{(2)}(x_{i+k})\end{aligned}$$

⇒ Prescribe conditions on  $\mathcal{E}_i$  to provide different sets of coefficients  $\mathbf{a}$  (i.e. different SEs).

# Structural Equations only based on accuracy

- step 1 Write the  $9 \times 9$  system such that  $\mathcal{E}_i(\mathbf{a}; \phi) = 0$  for  $\phi = (x - x_i)^m$ ,  $m = 0, \dots, 8$ .
- step 2 We derive the matrix system  $M\mathbf{a} = 0$  and  $\text{Ker}(M) = 0$ .
- step 3  $\text{Ker}(M[1 : 8, :])$  is a 1-dimension subspace with non-null vector  $\mathbf{a}_i^1$ . SEi1 equation is given by the non-degenerated equation

$$0 = \sum_{k=-1}^{k=1} a_{i,k}^{1,(0)} Z_{i+k} + \sum_{k=-1}^{k=1} a_{i,k}^{1,(1)} D_{i+k} + \sum_{k=-1}^{k=1} a_{i,k}^{1,(2)} S_{i+k}.$$

- ☞ For uniform mesh, we find again the first CCD of Chu-Fan equation and  $\mathbf{a}_i^1$  does not depend on  $i$ .

# Structural Equations only based on accuracy

step 4  $\text{Ker}(M[1 : 7, :])$  is a 2-dimension subspace that contains  $\mathbf{a}_i^1$ .  
We take  $\mathbf{a}_i^2$  orthogonal to  $\mathbf{a}_i^1$  and obtain SEi2.

$$0 = \sum_{k=-1}^{k=1} a_{i,k}^{2,(0)} Z_{i+k} + \sum_{k=-1}^{k=1} a_{i,k}^{2,(1)} D_{i+k} + \sum_{k=-1}^{k=1} a_{i,k}^{2,(2)} S_{i+k}.$$

☞ For uniform mesh, we find again the second CCD of Chu-Fan equation and  $\mathbf{a}_i^2 = \mathbf{a}^2$ .

☞ **We loose one-order!**

step 5 SEi3 derives from  $\text{Ker}(M[1 : 6, :])$  where  $\mathbf{a}_i^3$  is orthogonal to  $\mathbf{a}_i^1$  and  $\mathbf{a}_i^2$

☞ Does not exist in the C-F approach.

☞ **We loose one more order!**

# Solving 1D C-D-R problem

Assume we have a uniform mesh with constant  $\Delta x$ .

- PE1(i):  $-\kappa S_i + uD_i + rZ_i = f_i$ ,  $i = 0, \dots, I$ . Including  $i = 0$  and  $i = I$
- PE2(L):  $\alpha_L D_0 + \beta_L Z_0 = g(0)$
- PE2(R):  $\alpha_R D_I + \beta_R Z_I = g(1)$
- SE1(i):

$$15(Z_{i+1} - Z_{i-1}) - \Delta x(7D_{i+1} + 16D_i + 7D_{i-1}) + \Delta^2 x(S_{i+1} - S_{i-1}) = 0.$$

- SE2(i):

$$24(Z_{i+1} - 2Z_i + Z_{j-1}) - 9\Delta x(D_{i+1} - D_{i-1}) + \Delta^2 x(S_{i+1} - 8S_i + S_{i-1}) = 0.$$

- SE3(i):

$$8(Z_{i+1} - 2Z_i + Z_{j-1}) - 5\Delta x(D_{i+1} - D_{i-1}) + \Delta^2 x(S_{i+1} + S_{i-1}) = 0.$$

And now, we cook the scheme!

# Solving 1D C-D-R equation

- $i = 0$  we take PE1(0)+PE2(L)+SE3(1)
- $i = 1, \dots, I$ , we take PE1(i)+SE1(i)+SE2(i)
- $i = I$ , we take PE1(I)+PE2(R)+SE3(I-1)

Benchmark.  $\kappa = 1$ ,  $u = 1$ ,  $r = 1$ , exact solution  $\phi(x) = \exp(2x)$

☞ Dirichlet condition on both side ( $\alpha = 1$ ,  $\beta = 0$ )

I	err(Z)	order	err(D)	order	err(S)	order	cond
10	3,18E-09	***	1,92E-08	***	9,33E-09	***	2,93E+02
20	5,24E-11	5,9	3,37E-10	5,8	1,66E-10	5,8	5,96E+02
40	8,51E-13	5,9	5,58E-12	5,9	2,77E-12	5,9	1,60E+03
80	2,85E-14	4,9	2,38E-13	4,6	1,91E-12	5,4	6,40E+03

☞ Same order with other kind of boundary ( $\alpha = 0$ ,  $\beta = 1$ )

# Solving 1D Burger $\phi \phi' - \kappa \phi'' = f$

- PE1(i):  $Z_i D_i - \kappa S_i = f_i, i = 0, \dots, I.$
- PE2(L):  $\alpha_L D_0 + \beta_L Z_0 = g(0),$  PE2(R):  $\alpha_R D_I + \beta_R Z_I = g(1)$
- Same SE1, SE2, SE3

Fix point with a sequence of C-V  $Z_i^{[\ell]} D_i^{[\ell+1]} - \kappa S_i^{[\ell+1]} = f_i$

$\kappa = 1$

I	err(Z)	order	err(D)	order	err(S)	order
10	1,13E-08	***	1,77E-07	***	5,44E-08	***
20	2,06E-10	5,9	3,35E-09	5,7	1,31E-09	5,3
40	3,50E-12	5,9	5,87E-11	5,8	2,63E-11	5,6
60	7,19E-13	4,9	4,04E-12	6,6	6,19E-12	3,5
80	5,37E-12	***	4,54E-11	***	4,44E-11	***

$\kappa = 1/1000$

I	err(Z)	order	err(D)	order	err(S)	order
10	8,50E-11	***	1,17E-07	***	5,64E-07	***
20	1,40E-12	5,9	2,13E-09	5,7	1,38E-08	5,3
40	3,20E-14	5,4	3,54E-11	5,9	3,86E-10	5,1
60	1,29E-14	2,2	3,69E-12	5,5	9,98E-11	3,3
80	2,75E-14	***	2,34E-12	***	3,30E-10	***



## Some conclusions for the 1D space problem

- Very versatile schemes: choose your variables, your stencil and cook.
- $Z$ ,  $D$  and  $S$  have the same order, we do not lose accuracy for the 1st and 2nd derivatives.
- we do not have to compute the coefficients by hand but use the kernels to deduce the SEs.
- Trade-off between PEs and SEs: several options at the same point.
- A lot to say about diffusion/dispersion properties.
- 2D and 3D at least for structured grids.

# Structural method in time for EDO

We want to solve the scalar EDO equation

$$\phi'(t) = f(\phi(t), t), \quad \phi(0) = \phi_0.$$

We denote by  $t_n = n\Delta t$ ,  $n = 0, \dots$  and the approximations

- $Z_n \approx \phi(t_n)$ ,  $D_n \approx \phi'(t_n)$ ,  $S_n \approx \phi''(t_n)$
- Physical Equation PE1(n)  $D_n = f(Z_n, t_n)$
- Physical Equation PE2(n)  $S_n = \partial_z f(Z_n, t_n)D_n + \partial_t f(Z_n, t_n)$

☞ Build the Structural Equations.

# The one-point Z-D scheme ZD1

step 1 We introduce the functional

$$\mathcal{E}_n(\mathbf{a}; \phi) = a_0^{(0)} \phi(t_n) + a_1^{(0)} \phi(t_{n+1}) + a_0^{(1)} \phi'(t_n) + a_1^{(1)} \phi'(t_{n+1})$$

step 2 Build the  $4 \times 4$  matrix  $M$  such that we have  $\mathcal{E}_n(\mathbf{a}; \phi) = 0$  for  $\phi = (t - t_n)^m$ ,  $m = 0, 1, 2, 3$

step 3 Take the vector  $\mathbf{a} \in \ker(M[1 : 3, :])$  that gives the SE1

$$\frac{D_{n+1} + D_n}{2} - \frac{Z_{n+1} - Z_n}{\Delta t} = 0$$

☞ Coupling PE1 and SE1 provides the 2nd Crank-Nicholson Scheme.

# The two-points Z-D scheme ZD2

We use an intermediate point at  $t_{n+1/2}$ .

step 1 Two Physical Equations PE1, PE2:

$$D_{n+1/2} = f(Z_{n+1/2}, t_{n+1/2}), \quad D_{n+1} = f(Z_{n+1}, t_{n+1})$$

step 2 The (6 coefficients) functional is

$$\mathcal{E}_n(\mathbf{a}; \phi) = \sum_{k=0,1/2,1} \left[ a_k^{(0)} \phi(t_{n+k}) + a_k^{(1)} \phi'(t_{n+k}) \right]$$

step 3 Build  $M$  such that  $\mathcal{E}_n(\mathbf{a}; \phi) = 0$ ,  $\phi = (t - t_n)^m$ ,  
 $m = 0, \dots, 5$ .

step 4 Take vector  $\mathbf{a}^1 \in \ker(M[1 : 5, :])$ .

step 5 Take vector  $\mathbf{a}^2 \in \ker(M[1 : 4, :])$ , orthogonal to  $\mathbf{a}^1$ .

# The two-points Z-D scheme ZD2

We obtain two Structural Equations

$$0 = -\frac{Z_{n+1} - Z_n}{\Delta t} + \frac{D_n + 4D_{n+1/2} + D_{n+1}}{6}, \quad SE1$$

$$0 = -\frac{Z_n - 2Z_{n+1/2} + Z_{n+1}}{\Delta t} + \frac{D_{n+1} - D_n}{4}, \quad SE2$$

Given  $Z_n, D_n$ , we compute  $Z_{n+1/2}, D_{n+1/2}, Z_{n+1}, D_{n+1}$ , using SE1, SE2, PE1, PE2

## Main properties

The scheme is  $A$ -stable. No restriction on  $\Delta t$

The scheme is 4th-order both for  $Z$  and  $D$ .

☞ We find again the one-step implicit-block method: Shampine and Watts (1969,1972) and Axelsson (1969).

# The one-point Z-D-S scheme ZDS1

The unknowns are  $Z_{n+1}$ ,  $D_{n+1}$  and  $S_{n+1}$

**step 1** Two Physical Equations:  $D_{n+1} = f(Z_{n+1}, t_{n+1})$  PE1,  
 $S_{n+1} = \partial_z f(Z_{n+1}, t_{n+1})D_{n+1} + \partial_t f(Z_{n+1}, t_{n+1})$  PE2.

**step 2** The (6 coefficients) functional is

$$\mathcal{E}_n(\mathbf{a}; \phi) = \sum_{k=0,1} \left[ a_k^{(0)} \phi(t_{n+k}) + a_k^{(1)} \phi'(t_{n+k}) + a_k^{(2)} \phi''(t_{n+k}) \right]$$

**step 3** Build  $M$  such that  $\mathcal{E}_n(\mathbf{a}; \phi) = 0$ ,  $\phi = (t - t_n)^m$ ,  
 $m = 0, \dots, 5$ .

**step 4** Take vector  $\mathbf{a}^1 \in \ker(M[1 : 5, :])$ .

# The one-point Z-D-S scheme ZDS1

We obtain one Structural Equation SE1

$$0 = 12(Z_n - Z_{n+1}) + 6\lambda\Delta t(Z_n + Z_{n+1}) + (\lambda\Delta t)^2(Z_n - Z_{n+1}).$$

Given  $Z_n$ ,  $D_n$ , we compute  $Z_{n+1}$ ,  $D_{n+1}$ ,  $S_{n+1}$  using SE1, PE1, PE2

## Main properties

The scheme is  $A$ -stable. No restriction on  $\Delta t$

The scheme is 4th-order for  $Z$ ,  $D$ , and  $S$ . Less equations to solve, but the price is the new Physical Equation (hence more non-linear)

☞ We find again the multistep multi-derivative method: Lambert and Mitchell (1962, 1963).



# The two-points Z-D-S scheme ZDS2

Unknowns are  $Z_{n+1/2}$ ,  $D_{n+1/2}$ ,  $S_{n+1/2}$  and  $Z_{n+1}$ ,  $D_{n+1}$ ,  $S_{n+1}$

step 1 4 Physical Equations.

step 2 A (9 coefficients) functional

step 3 Build  $M$  such that  $\mathcal{E}_n(\mathbf{a}; \phi) = 0$ ,  $\phi = (t - t_n)^m$ ,  
 $m = 0, \dots, 8$ .

step 4 Take vector  $\mathbf{a}^1 \in \ker(M[1 : 8, :])$ .

step 5 Take vector  $\mathbf{a}^2 \in \ker(M[1 : 7, :])$ , orthogonal to  $\mathbf{a}^1$ .

# The two-points Z-D-S scheme ZDS2

We obtain two Structural Equation SE1, SE2

$$0 = 16 \frac{Z_{n+1} - 2Z_{n+1/2} + Z_n}{(\Delta t)^2} - 3 \frac{D_{n+1} - D_n}{\Delta t} + \frac{S_{n+1} - 8S_{n+1/2} + S_n}{6}$$
$$0 = 30 \frac{Z_{n+1} - Z_n}{(\Delta t)^2} - \frac{7D_{n+1} + 16D_{n+1/2} + 7D_n}{\Delta t} + \frac{S_{n+1} - S_n}{2}.$$

Given  $Z_n, D_n, S_n$  we compute the 6 unknowns using SE1, SE2, PE1, PE2, PE3, PE4

## Main properties

The scheme is linearly unconditional stable. No restriction on  $\Delta t$

The scheme is 6th-order for  $Z, D$ , and  $S$ .

☞ We find again the multi-derivative implicit-block method (Enright 1974, Sahi, Jator, Khan 2012 Ehigie 2014).

# A genuine two-points Z-D-S scheme NZDS

☞ All the traditional schemes systematically substitute  $D$  and  $S$  by the PEs: 2 SEs and 4 PEs.

We design a scheme with 4 SEs and 2 PEs (no equivalent in EDO)

$$0 = 16 \frac{Z_{n+1} - 2Z_{n+1/2} + Z_n}{(\Delta t)^2} - 3 \frac{D_{n+1} - D_n}{\Delta t} + \frac{S_{n+1} - 8S_{n+1/2} + S_n}{6},$$

$$0 = 30 \frac{Z_{n+1} - Z_n}{(\Delta t)^2} - \frac{7D_{n+1} + 16D_{n+1/2} + 7D_n}{\Delta t} + \frac{S_{n+1} - S_n}{2},$$

$$0 = -8 \frac{Z_{n+1} - 2Z_{n+1/2} + Z_n}{(\Delta t)^2} + \frac{D_{n+1} - D_n}{\Delta t} + S_{n+1/2},$$

$$0 = 12 \frac{Z_{n+1} - Z_n}{(\Delta t)^2} - 2 \frac{D_{n+1} + 4D_{n+1/2} + D_n}{\Delta t},$$

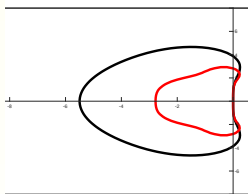
$$D_{n+1} = f(Z_{n+1}), \quad D_{n+1/2} = f(Z_{n+1/2}).$$

☞ No Physical equation for  $S$ .

## Main properties

The scheme is conditionally stable but with a larger stability region w.r. to RK4

The scheme is 4th-order for  $Z$ ,  $D$ , and  $S$ .



➡ Additional note: with the Kernel technique, time step can be non-uniform.

$$\phi' + \lambda\phi = f(t), \quad \phi(0) = \phi_0, \lambda \in \mathbb{R}$$

time scheme	N	Z		D		S	
		errZ	ord	errD	ord	errS	ord
2ZD	2	3.24E-05	---	3.24E-05	---		
	4	2.00E-06	4.02	2.00E-06	4.02		
	6	3.95E-07	4.01	3.95E-07	4.01		
	8	1.25E-07	4.00	1.25E-07	4.00		
1ZDS	2	3.24E-05	---	3.24E-05	---	3.24E-05	---
	4	2.00E-06	4.02	2.00E-06	4.02	2.00E-06	4.02
	6	3.95E-07	4.01	3.95E-07	4.01	3.95E-07	4.01
	8	1.25E-07	4.00	1.25E-07	4.00	1.25E-07	4.00
2ZDS	2	9.64E-09	---	9.64E-09	---	9.64E-09	---
	4	1.49E-10	6.02	1.49E-10	6.02	1.49E-10	6.02
	6	1.31E-11	6.01	1.31E-11	6.01	1.31E-11	6.01
	8	2.32E-12	6.00	2.32E-12	6.00	2.32E-12	6.00
NZDS	2	1.08E-05	---	1.08E-05	---	1.08E-05	---
	4	5.82E-07	4.22	5.82E-07	4.22	5.82E-07	4.22
	6	1.09E-07	4.13	1.09E-07	4.13	1.09E-07	4.13
	8	3.37E-08	4.09	3.37E-08	4.09	3.37E-08	4.09

$$\phi' + i2k\pi\phi = f(t), \quad \phi(0) = \phi_0, \quad k = 10$$

time scheme	N	Z		D		S	
		err	ord	err	ord	err	ord
2ZD	10	1.80E+00	---	5.67E+01	---		
	20	2.27E-01	2.99	7.13E+00	2.99		
	30	4.91E-02	3.78	1.54E+00	3.78		
	40	1.60E-02	3.90	5.02E-01	3.90		
1ZDS	10	1.80E+00	---	5.67E+01	---	1.78E+03	---
	20	2.27E-01	2.99	7.13E+00	2.99	2.24E+02	2.99
	30	4.91E-02	3.78	1.54E+00	3.78	4.84E+01	3.78
	40	1.60E-02	3.90	5.02E-01	3.90	1.58E+01	3.90
2ZDS	10	2.64E-02	---	8.29E-01	---	2.61E+01	---
	20	6.74E-04	5.29	2.12E-02	5.29	6.65E-01	5.29
	30	6.42E-05	5.80	2.02E-03	5.80	6.34E-02	5.80
	40	1.18E-05	5.90	3.69E-04	5.90	1.16E-02	5.90
NZDS	10	1.94E+00	---	6.11E+01	---	1.92E+03	---
	20	7.31E-02	4.73	2.30E+00	4.73	7.22E+01	4.73
	30	1.37E-02	4.13	4.30E-01	4.13	1.35E+01	4.13
	40	4.25E-03	4.06	1.34E-01	4.06	4.20E+00	4.06

# Non linear (stiff) case

Sigmoid  $\phi(t) = \frac{1}{1 + e^{-\lambda t}}$  of  $\phi' = \lambda\phi(\phi - 1)$ ,  $\phi_0 = \phi(-1)$ .

time scheme	$N$	$Z$		$D$		$S$	
		$\lambda = 5$	err	ord	err	ord	err
2ZD	20	4.61E-02	---	7.40E+00	---		
	30	1.46E-02	2.83	1.57E+00	3.83		
	40	5.06E-03	3.70	5.08E-01	3.91		
	60	1.04E-03	3.90	1.02E-01	3.95		
1ZDS	20	4.61E-02	---	7.40E+00	---	4.64E+01	---
	30	1.46E-02	2.83	1.57E+00	3.83	1.47E+01	2.83
	40	5.06E-03	3.70	5.08E-01	3.91	5.09E+00	3.7
	60	1.04E-03	3.90	1.02E-01	3.95	1.05E+00	3.90
2ZDS	20	2.23E-04	---	2.17E-02	---	2.24E-01	---
	30	2.13E-05	5.79	2.07E-03	5.79	2.14E-02	5.79
	40	3.89E-06	5.90	3.80E-04	5.90	3.92E-03	5.90
	60	3.49E-07	5.95	3.41E-05	5.95	3.51E-04	5.95
2ZDS	10	4.81E-05	5.02	1.11E-04	6.12	7.69E-02	3.03
	20	3.04E-06	3.99	7.02E-06	3.99	1.85E-02	2.05
	30	6.01E-07	4.00	1.45E-06	3.88	8.17E-03	2.02
	40	1.90E-07	4.00	4.67E-07	3.95	4.58E-03	2.01

# The (time) structural method for PDE



Consider the PDE

$$\partial_t \phi - \kappa \partial_{xx} \phi + u \partial_x \phi = f$$

with **periodic** boundary conditions.

- $A_c \phi$  the 6th/8th order finite difference discretization of  $\partial_x \phi$
- $A_d \phi$  the 6th/8th order finite difference discretization of  $\partial_{xx} \phi$
- Semi-discrete problem

$$\partial_t Z(t) - \kappa A_d Z(t) + u A_d Z(t) = F(t)$$

with  $Z(t) = [Z_1(t), \dots, Z_I(t)]^T$ .

- With the same notations for  $D(t)$  and  $S(t)$ , we have two Physical Equations

$$D(t) = \kappa A_d Z(t) - u A_d Z(t) + F(t), \quad PE1$$

$$S(t) = \kappa A_d D(t) - u A_d D(t) + F'(t), \quad PE2$$

# Time discretization with Structural Equations

We present the ZDS1 case as an example.

For the EDO case, the structural equation reads

$$0 = 12(Z_n - Z_{n+1}) + 6\lambda\Delta t(D_n + D_{n+1}) + (\lambda\Delta t)^2(S_n - S_{n+1}).$$

We use exactly the same equation but as a vector with

$$Z_n = [Z_{n,1}, \dots, Z_{n,I}]^T$$

We solve the  $3I$  system composed of PE1, PE2 and SE1.

☞ All the three schemes are unconditionally stable.

# Benchmark pure convection equation

$$\partial_t \phi - \partial_x \phi = f$$

	N	Z				D				S			
		E1	O1	E00	O00	E1	O1	E00	O00	E1	O1	E00	O00
2D	20	6.76E-05	---	1.06E-04	---	4.25E-04	---	6.68E-04	---				
	25	2.78E-05	3.99	4.37E-05	3.99	1.74E-04	3.99	2.74E-04	3.99				
	30	1.34E-05	3.99	2.11E-05	3.99	8.42E-05	3.99	1.33E-04	3.99				
	35	7.24E-06	3.99	1.14E-05	3.99	4.55E-05	3.99	7.16E-05	3.99				
1ZDS	20	1.96E-04	---	3.08E-04	---	1.23E-03	---	1.94E-03	---	7.73E-03	---	1.22E-02	---
	25	8.04E-05	3.99	1.27E-04	3.99	5.05E-04	3.99	7.95E-04	3.99	3.18E-03	3.99	5.00E-03	3.99
	30	3.88E-05	3.99	6.11E-05	3.99	2.44E-04	3.99	3.84E-04	3.99	1.53E-03	3.99	2.41E-03	3.99
	35	2.10E-05	3.99	3.30E-05	3.99	1.32E-04	3.99	2.08E-04	3.99	8.28E-04	3.99	1.30E-03	3.99
2ZDS	20	1.02E-07	---	1.60E-07	---	6.38E-07	---	1.00E-06	---	4.00E-06	---	6.30E-06	---
	25	2.65E-08	6.02	4.18E-08	6.02	1.66E-07	6.03	2.61E-07	6.03	1.04E-06	6.05	1.63E-06	6.06
	30	8.77E-09	6.08	1.38E-08	6.08	5.45E-08	6.11	8.56E-08	6.12	3.35E-07	6.19	5.27E-07	6.19
	35	3.36E-09	6.22	5.29E-09	6.22	2.06E-08	6.33	3.22E-08	6.33	1.26E-07	6.33	1.99E-07	6.33

# Benchmark CD equation

$$\partial_t \phi - \partial_{xx} \phi - \partial_x \phi = f$$

	N	Z				D				S			
		E1	O1	E00	O00	E1	O1	E00	O00	E1	O1	E00	O00
RK4	40	NaN	---	NaN	---								
	3700	NaN	---	NaN	---								
	3800	6.24E-11	---	9.81E-11	---								
2D	40	1.25E-05	---	1.96E-05	---	4.92E-04	---	7.73E-04	---				
	3700	7.08E-11	2.67	1.11E-10	2.67	9.30E-10	2.91	1.46E-09	2.91				
	3800	7.06E-11	0.09	1.11E-10	0.08	9.29E-10	0.05	1.46E-09	0.05				
1ZDS	40	3.33E-06	---	5.22E-06	---	1.31E-04	---	2.06E-04	---	5.18E-03	---	8.14E-03	---
	3700	7.06E-11	2.38	1.11E-10	2.38	9.33E-10	2.62	1.47E-09	2.62	1.24E-08	2.86	2.34E-08	2.82
	3800	7.04E-11	0.09	1.11E-10	0.07	9.31E-10	0.07	1.47E-09	0.06	1.24E-08	↑	2.47E-08	↑
2ZDS	40	4.45E-10	---	6.99E-10	---	1.64E-08	---	2.57E-08	---	6.82E-07	---	1.07E-06	---
	3700	7.06E-11	0.41	1.11E-10	0.41	9.31E-10	0.63	1.47E-09	0.63	1.24E-08	0.89	2.41E-08	0.84
	3800	7.04E-11	0.09	1.11E-10	0.07	9.30E-10	0.07	1.46E-09	0.05	1.23E-08	0.28	2.44E-08	↑

# Benchmark Schrödinger equation

$$\partial_t \phi(t, x) - i \partial_{xx} \phi(t, x) = f$$

	H	Z				D				S			
		E1	O1	E00	O00	E1	O1	E00	O00	E1	O1	E00	O00
2ZD	30	3.74E-05	---	3.61E-04	---	2.47E-04	---	2.47E-03	---				
	40	1.26E-05	3.80	1.16E-04	3.93	8.48E-05	3.71	8.02E-04	3.92				
	50	5.28E-06	3.89	4.83E-05	3.95	3.60E-05	3.84	3.33E-04	3.94				
	60	2.58E-06	3.93	2.35E-05	3.96	1.77E-05	3.90	1.62E-04	3.95				
	70	1.41E-06	3.94	1.27E-05	3.96	9.66E-06	3.92	8.81E-05	3.95				
1ZDS	30	3.74E-05	---	3.61E-04	---	2.47E-04	---	2.47E-03	---	1.87E-03	---	1.97E-02	---
	40	1.26E-05	3.80	1.16E-04	3.93	8.48E-05	3.71	8.01E-04	3.92	6.62E-04	3.61	6.40E-03	3.91
	50	5.28E-06	3.89	4.83E-05	3.95	3.60E-05	3.84	3.33E-04	3.94	2.84E-04	3.78	2.67E-03	3.92
	60	2.58E-06	3.93	2.35E-05	3.96	1.77E-05	3.90	1.62E-04	3.95	1.41E-04	3.86	1.30E-03	3.94
	70	1.41E-06	3.94	1.27E-05	3.96	9.66E-06	3.92	8.81E-05	3.95	7.70E-05	3.90	7.08E-04	3.95
2ZDS	30	6.26E-08	---	5.89E-07	---	5.61E-07	---	5.29E-06	---	5.58E-06	---	5.27E-05	---
	40	8.80E-09	6.82	8.53E-08	6.72	8.48E-08	6.56	8.18E-07	6.49	9.00E-07	6.34	8.61E-06	6.30
	50	2.73E-09	5.25	2.53E-08	5.44	1.78E-08	7.01	1.41E-07	7.88	1.57E-07	7.82	1.22E-06	8.75
	60	3.84E-09	↑	3.68E-08	↑	2.41E-08	↑	2.36E-07	↑	1.73E-07	↑	1.74E-06	↑
	70	4.48E-09	↑	4.13E-08	↑	2.97E-08	↑	2.78E-07	↑	2.29E-07	↑	2.16E-06	↑

# Benchmark wave system

$$\partial_t \phi + \partial_x \psi = 0 \quad \partial_t \psi + \partial_x \phi = F$$

	N	Z				D				S			
		E1	O1	E <sub>00</sub>	O <sub>00</sub>	E1	O1	E <sub>00</sub>	O <sub>00</sub>	E1	O1	E <sub>00</sub>	O <sub>00</sub>
2ZD	20	1.46E-01	---	2.27E-01	---	4.54E+00	---	7.13E+00	---				
	40	1.02E-02	3.83	1.60E-02	3.83	3.20E-01	3.83	5.02E-01	3.83				
	80	6.54E-04	3.96	1.03E-03	3.96	2.06E-02	3.96	3.23E-02	3.96				
	160	4.12E-05	3.99	6.47E-05	3.99	1.29E-03	3.99	2.03E-03	3.99				
1ZDS	20	1.46E-01	---	2.27E-01	---	4.54E+00	---	7.13E+00	---	1.43E+02	---	2.24E+02	---
	40	1.02E-02	3.83	1.60E-02	3.83	3.20E-01	3.83	5.02E-01	3.83	1.00E+01	3.83	1.58E+01	3.83
	80	6.54E-04	3.96	1.03E-03	3.96	2.06E-02	3.96	3.23E-02	3.96	6.46E-01	3.96	1.01E+00	3.96
	160	4.12E-05	3.99	6.47E-05	3.99	1.29E-03	3.99	2.03E-03	3.99	4.06E-02	3.99	6.39E-02	3.99
2ZDS	20	4.29E-04	---	6.74E-04	---	1.35E-02	---	2.12E-02	---	4.23E-01	---	6.65E-01	---
	40	7.48E-06	5.84	1.18E-05	5.84	2.35E-04	5.84	3.69E-04	5.84	7.39E-03	5.84	1.16E-02	5.84
	80	1.20E-07	5.96	1.89E-07	5.96	3.77E-06	5.96	5.93E-06	5.96	1.19E-04	5.96	1.86E-04	5.96
	160	1.89E-09	5.99	2.97E-09	5.99	5.94E-08	5.99	9.33E-08	5.99	1.87E-06	5.99	2.93E-06	5.99

# Benchmark Burger equation

$$\partial_t u - u \partial_x u = f$$

	N	$\bar{k}$	Z				D				S			
			E1	O1	E00	O00	E1	O1	E00	O00	E1	O1	E00	O00
2D	30	11.00	1.87E-05	---	4.39E-05	---	1.76E-04	---	4.13E-04	---				
	40	10.00	5.87E-06	4.03	1.38E-05	4.02	5.51E-05	4.03	1.31E-04	3.99				
	50	10.00	2.40E-06	4.02	5.64E-06	4.02	2.25E-05	4.02	5.35E-05	4.00				
	60	9.00	1.15E-06	4.01	2.71E-06	4.01	1.08E-05	4.01	2.58E-05	4.00				
1ZDS	30	13.00	3.43E-05	---	7.03E-05	---	2.17E-04	---	4.60E-04	---	3.57E-03	---	1.24E-02	---
	40	12.00	1.08E-05	4.00	2.22E-05	4.00	6.87E-05	4.00	1.46E-04	4.00	1.13E-03	3.99	3.95E-03	3.99
	50	11.00	4.43E-06	4.00	9.10E-06	4.00	2.81E-05	4.00	5.97E-05	4.00	4.65E-04	3.99	1.62E-03	4.00
	60	11.00	2.14E-06	4.00	4.39E-06	4.00	1.36E-05	4.00	2.88E-05	4.00	2.25E-04	4.00	7.81E-04	3.99
2D	30	11.97	7.91E-09	---	1.63E-08	---	5.01E-08	---	1.07E-07	---	8.29E-07	---	2.89E-06	---
	40	11.00	1.40E-09	6.01	2.89E-09	6.01	8.91E-09	6.01	1.89E-08	6.01	1.47E-07	6.00	5.13E-07	6.00
	50	10.98	3.68E-10	6.00	7.56E-10	6.01	2.33E-09	6.00	4.96E-09	6.01	3.87E-08	6.00	1.35E-07	5.99
	60	10.00	1.23E-10	6.00	2.53E-10	6.00	7.81E-10	6.00	1.66E-09	6.01	1.29E-08	6.00	4.51E-08	6.00

# Benchmark Euler system

$$f = \partial_t \rho + \partial_x m, \quad g = \partial_t m + \partial_x (2\varepsilon + p), \quad h = \partial_t E + \partial_x (u(E + p))$$

	$N$	$\bar{k}$	$Z_\rho$				$D_\rho$				$S_\rho$			
			E1	O1	E00	O00	E1	O1	E00	O00	E1	O1	E00	O00
2D	10	9.00	8.30E-06	---	3.26E-05	---	9.32E-05	---	4.44E-04	---				
	15	8.20	1.65E-06	3.99	6.49E-06	3.98	1.85E-05	3.98	9.03E-05	3.93				
	20	7.70	5.21E-07	4.00	2.06E-06	3.99	5.88E-06	3.99	2.88E-05	3.97				
	25	7.40	2.14E-07	4.00	8.43E-07	4.00	2.41E-06	4.00	1.18E-05	3.99				
1ZDS	10	9.50	9.77E-06	---	1.78E-05	---	3.59E-05	---	1.45E-04	---	3.77E-04	---	1.51E-03	---
	15	8.80	1.93E-06	4.00	3.52E-06	4.00	7.12E-06	3.99	2.92E-05	3.96	7.51E-05	3.98	3.07E-04	3.93
	20	8.40	6.11E-07	4.00	1.11E-06	4.00	2.26E-06	3.99	9.29E-06	3.98	2.38E-05	3.99	9.80E-05	3.97
	25	8.00	2.50E-07	4.00	4.56E-07	4.00	9.25E-07	4.00	3.81E-06	3.99	9.77E-06	3.99	4.03E-05	3.98
2ZDS	10	8.60	7.26E-10	---	1.32E-09	---	2.67E-09	---	1.10E-08	---	2.81E-08	---	1.17E-07	---
	15	8.07	6.39E-11	6.00	1.16E-10	5.99	2.34E-10	6.00	9.61E-10	6.00	2.47E-09	6.00	1.02E-08	6.00
	20	7.80	1.14E-11	5.99	2.09E-11	5.97	4.07E-11	6.08	1.64E-10	6.15	4.29E-10	6.08	1.80E-09	6.04
	25	7.56	3.03E-12	5.93	5.68E-12	5.83	1.03E-11	6.17	4.22E-11	6.08	1.57E-10	4.49	5.78E-10	5.09



- Theoretical aspect (stability non linear, convergence)
- Connection with EDO scheme (generalized multi linear methods)
- Structural equation in time AND space
- Use other constrains than the accuracy (spectral resolution)
- 2D and 3D in space
- Generalized finite difference method on clouds
- Shock and discontinuities