FREEFEM'14, December, 11, UPMC

A FINITE ELEMENT METHOD FOR AN ILL-POSED OXYGEN-BALANCE MODEL

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EUTROPHICATION

Excess of Organic matter \Longrightarrow Excess of nutrients \Longrightarrow Eutrophication





Le Thouet (F.), Cunnning River (Australia) (Source: WEB!).

Travail en collaboration avec

- LJLL, Paris 6 (C. Bernardi, F. Hecht)
- I2M, Bordeaux I (M. Azaïez, C. Lebot)
- LMA, Reims (S. Salmon)
- ICJ, Lyon I (N. Débit)
- LAMSIN, Tunis (H. EL Fekih)
- LMAC Compiègne (M. Andrle, S. Khiari)

BOD Model

Organic Pollution in a body of water (\Longrightarrow) b: Biochemical Oxygen Demand (BOD).

Reaction (Streeter & Phelps, 1925). (Notation: Ω domaine, dim ≥ 2)

$$\frac{\partial_t b}{\partial t} + Rb = F$$
 in $\Omega \times (0, T)$.

Transport in the River

$$\frac{\partial_t b}{\partial t} + \operatorname{div}(Vb) + Rb = F \quad \text{in } \Omega \times (0, T),$$

Dispersion of Oxygen in water

$$\frac{\partial_t b}{\partial t} - \operatorname{div}(D\nabla b) + \operatorname{div}(Vb) + Rb = F$$
 in $\Omega \times (0, T)$.

DO Model

c: Dissolved Oxygen concentration

 c_S : Dissolved Oxygen concentration at saturation (constant)

Pump out Oxygen (⇒) Oxygen Deficit

(⇒) Oxygen Absorption from Atmosphere

(Dispersion, Transport, Reaction)

$$\partial_t c - \operatorname{div}(D\nabla c) + \operatorname{div}(Vc) + R_*c = G$$
 in $\Omega \times (0, T)$.

BOD-DO Model

Organic Pollution Source (F), Oxygen Source (G)

$$\partial_t b - \operatorname{div} (D\nabla b) + \operatorname{div} (Vb) + Rb = F \qquad \text{in } \Omega \times (0, T),$$

$$\partial_t c - \operatorname{div} (D\nabla c) + \operatorname{div} (Vc) + R_*c + Rb = G \qquad \text{in } \Omega \times (0, T),$$

$$D\partial_{\boldsymbol{n}} b = \gamma \qquad \text{in } \partial\Omega \times (0, T),$$

$$D\partial_{\boldsymbol{n}} c = 0 \qquad \text{in } \partial\Omega \times (0, T),$$

$$b(0) = 0 \qquad \text{in } \Omega,$$

$$c(0) = c_S \qquad \text{in } \Omega.$$

Manuscripts: Brown (EPA, 1987), Okubo (Springer, 1980). Wider (Huge) Bibliography in this model.

STREETER-PHELPS MODEL (1925)

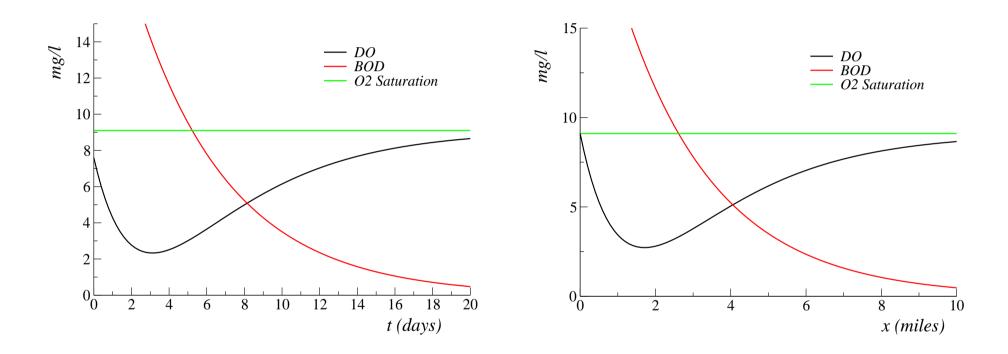


Diagram to the left: Initial pollution, (No Dispersion nor Advection)

Diagram to the right: Steady pollution, (No Dispersion).

Observations on BOD or on DO?

Obtain Experimentally $\gamma (= \partial_{\boldsymbol{n}} b)$

Long Chemical Protocol
$$(\Longrightarrow)$$
 Measurments of the BOD flux γ (\Longrightarrow) Lasts five Days! Too Long!

Observations $c (= \alpha)$

Use the observations $D\partial_n c$ and c on the bondary, available in real-time and directly cope with the inverse Coupled BOD-DO system.

INVERSE BOD-DO MODEL

No boundary condition for b on Γ_C .

Two boundary conditions for c on Γ_C .

$$\partial_t b - \operatorname{div} (D\nabla b) + [\operatorname{div} (Vb)] + Rb = F \qquad \text{in } \Omega \times (0, T),$$

$$\partial_t c - \operatorname{div} (D\nabla c) + [\operatorname{div} (Vc)] + R_*c + Rb = G \qquad \text{in } \Omega \times (0, T),$$

$$D\partial_n c = 0 \qquad \text{in } \partial\Omega \times (0, T),$$

$$c = \alpha, \qquad \text{in } \partial\Omega \times (0, T),$$

$$b(0) = 0, \qquad \text{in } \Omega,$$

$$c(0) = c_S \qquad \text{in } \Omega.$$

The flux (the load) to reconstruct:

$$(D\partial_{\boldsymbol{n}}b)(t)|_{\partial\Omega} = \gamma? \text{ (or } b(t)|_{\partial\Omega} = \eta?) \text{ in } (0,T).$$

Ill-posedness (1D Model)

Consider $\gamma(t) = Db'(0,t)$ as unknown. Solve sequentially

$$\partial_t b_{\gamma} - (Db'_{\gamma})' + Rb_{\gamma} = 0 \qquad \text{in } (0, \pi) \times (0, T),$$

$$Db'_{\gamma}(0, t) = 0, \qquad \text{in } (0, T),$$

$$Db'_{\gamma}(\pi, t) = \gamma(t), \qquad \text{in } (0, T),$$

$$b_{\gamma}(0, \cdot) = 0, \qquad \text{in } (0, \pi).$$

$$\partial_t c_{\gamma} - (Dc'_{\gamma})' + R_* c_{\gamma} = Rb_{\gamma} \qquad \text{in } (0, \pi) \times (0, T),$$

$$Dc'_{\gamma}(0, t) = 0, \qquad \text{in } (0, T),$$

$$Dc'_{\gamma}(\pi, t) = 0, \qquad \text{in } (0, T),$$

$$c_{\gamma}(0, \cdot) = 0, \qquad \text{in } (0, T),$$

$$c_{\gamma}(0, \cdot) = 0, \qquad \text{in } (0, \pi).$$

We have to solve the ill-posed equation on $\gamma \in L^2(0,T)$, that is

$$S\gamma(t) = c_{\gamma}(\pi, t) = \alpha(t),$$
 in $(0, T)$.

Ill-posedness (II)

Fourier Computations ($D = R = R_* = 1$)

$$b_{\gamma}(x,t) = \frac{2}{\pi} \sum_{k \in \mathbb{N}} \left(\int_0^t \gamma(s) e^{-k^2(t-s)} ds \right) \cos(kx),$$

$$c_{\gamma}(x,t) = \frac{2}{\pi} \sum_{k \in \mathbb{N}} \left(\int_0^t \gamma(s) (t-s) e^{-k^2(t-s)} ds \right) \cos(kx),$$

$$(S\gamma)(t) = \int_0^t K(t-s)\gamma(s) ds, \qquad \forall t \in (0,T),$$

$$K(s) = \frac{1}{\pi}s + \frac{2}{\pi} \sum_{k \in \mathbb{N}} se^{-k^2 s}, \quad \forall s \in (0, T).$$

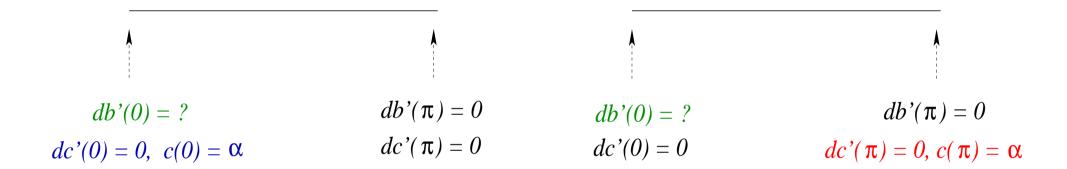
 $K(s) = \mathcal{O}(\sqrt{s}) \iff$ Singular values of S decrease like $k^{-3/2}$.

 $(S\gamma = \alpha)$ is a mildly ill-posed Volterra equation.

Why the MILD Ill-posedness?

Observation loc. = Reconstruction l.

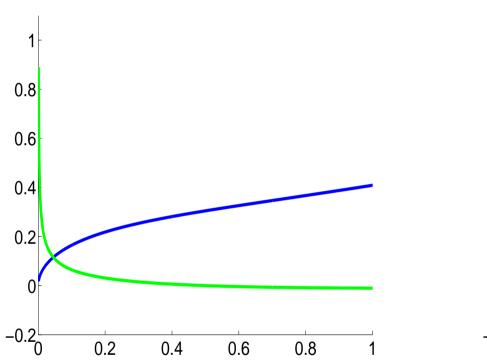
Observa. loc. \neq Reconstruc. loc.

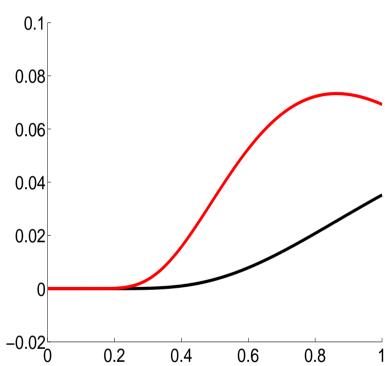


Kernels of Volterra Equations (replace 2 by 1 for k = 0)

$$K(s) = \frac{s}{\pi} + \frac{2s}{\pi} \sum_{k \ge 1} e^{-k^2 s},$$
 $H(s) = \frac{s}{\pi} + \frac{2s}{\pi} \sum_{k \ge 1} (-1)^k e^{-k^2 s}.$

CONVOLUTION KERNELS





Kernels $K(\cdot)$ and $H(\cdot)$ and their first derivatives !! Different scales in the vertical axis.

Uniqueness: Illustration $(T = \infty)$

Solve equation

$$(S\gamma)(t) = K \star \gamma(t) = 0 \quad \forall t \in (0, \infty).$$

Use Laplace transform yields that

$$\widehat{K}(p)\widehat{\gamma}(p) = 0, \quad \forall p \in (0, \infty),$$

The Laplace Transform of $K(\cdot)$ is

$$\widehat{K}(p) = \frac{2}{\xi} \sum_{k \in \mathbb{N}} \frac{1}{(p + \lambda_k)^2} > 0, \quad \forall p \in (0, \infty).$$

We obtain then that

$$(\hat{\gamma}(p) = 0, \ \forall p \in (0, \infty)) \implies (\gamma(t) = 0, \ \forall t \in (0, \infty)).$$

Then

$$b(t,x) = c(t,x) = 0, \qquad \forall t \in (0,\infty), \ \forall x \in (0,L).$$

A Uniqueness Result

THÉO. 1 The Inverse Problem has at most one solution.

PROOF

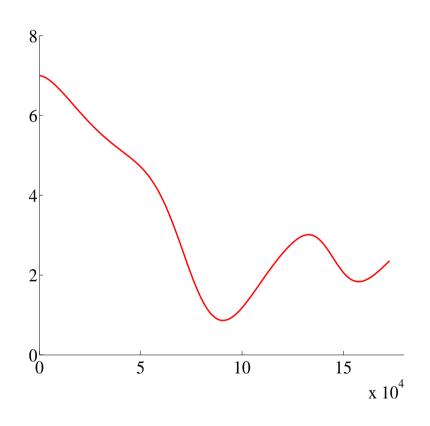
i — Study of the resolvant of the steady problem : Saddle point theory for non symmetric problems (Nicolaides & Bernardi, Canuto, Maday).

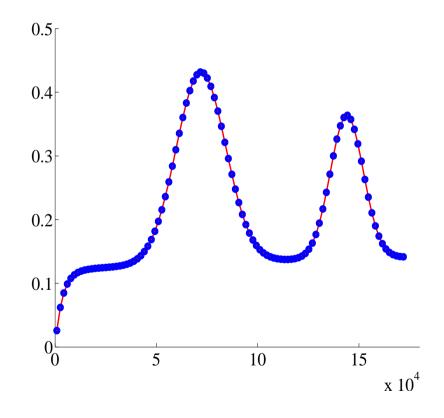
ii — Then, use the uniqueness theorem for parabolic problems (A. Pazy).

Details in M3AS, Volume 22, Issue 10, October 2012

Numerics (I): Volterra's equation

Computations based on the MATLAB Library regu developed by P. C. Hansen, http://www.imm.dtu.dk/~pcha

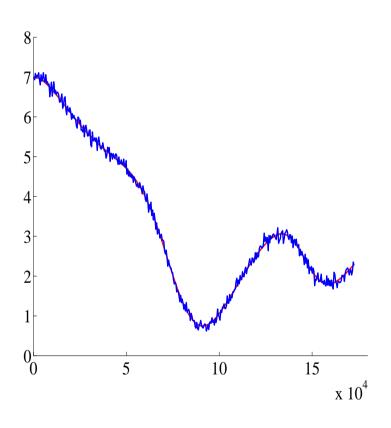


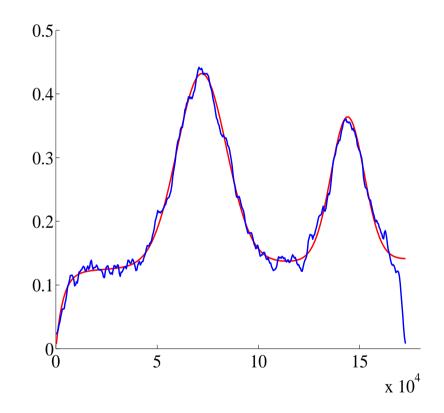


Unnoisy Observation $\alpha(\cdot)$.

Exact and computed fluxes $\gamma(\cdot)$.

Gaussian Noise. Variance $\sigma=0.1$

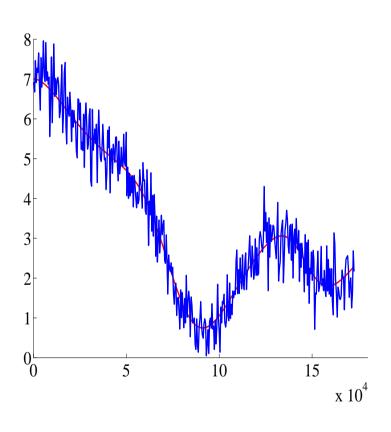


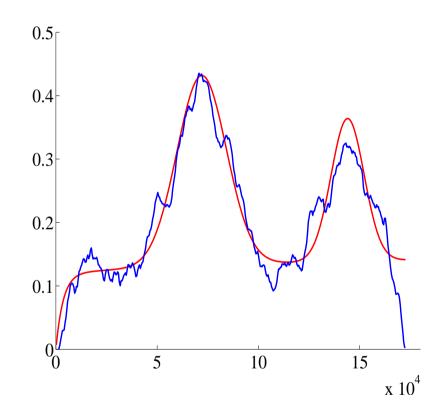


Noisy Observation $\alpha(\cdot)$.

Exact and computed fluxes $\gamma(\cdot)$.

Gaussian Noise. Variance $\sigma = 0.5$





Exact data Observation $\alpha(\cdot)$.

Exact and computed fluxes $\gamma(\cdot)$

Numerics: Steady Model

Ben B., Bernardi, Hecht, Salmon, (FREEFEM)

SIAM J. Numerical Analysis, 52-5 (2014), pp. 2207-2226

STEADY SYSTEM

Cancel every thing that is time dependence (\Longrightarrow)

$$-\operatorname{div}(D\nabla b) + Rb = F \qquad \text{in } \Omega$$

$$-\operatorname{div}(D\nabla c) + R_*c + Rb = G \qquad \text{in } \Omega,$$

$$D\partial_{\boldsymbol{n}}c = 0 \qquad \text{in } \partial\Omega,$$

$$c = \alpha, \qquad \text{in } \partial\Omega.$$

Looks like the Vorticity-Stream functions system in Incompressible Fluid Mechanic.

Difference: A Non-symmetric saddle point problem.

MIXED FINITE ELEMENTS $\mathcal{P}_1 \times \mathcal{P}_1$

 b_h and φ_h , no boundary conditions along $\partial\Omega$. c_h and ψ_h , Dirichlet conditions along $\partial\Omega$ ($c_h = \alpha_h$ and $\psi_h = 0$ on $\partial\Omega$.).

Find b_h and c_h such that

$$\int_{\Omega} (D\nabla b_{h} \nabla \psi_{h} + R b_{h} \psi_{h}) dx = \int_{\Omega} f \psi_{h} dx, \qquad \forall \psi_{h}$$

$$\int_{\Omega} (D\nabla \varphi_{h} \nabla c_{h} + R_{*} \varphi_{h} c_{h}) dx + \int_{\Omega} R b_{h} \varphi_{h} dx = \int_{\Omega} g \varphi_{h} dx, \qquad \forall \varphi_{h}$$

'Abstract form'

$$\kappa (\psi_h, b_h) = (f, \psi_h), \qquad \forall \psi_h,$$

$$\kappa_*(c_h, \varphi_h) + a(b_h, \varphi_h) = (g, \varphi_h), \qquad \forall \varphi_h$$

THEORETICAL RESULTS

inf-sup condition on $\kappa(\cdot, \cdot)$ (\Longrightarrow) OK! inf-sup condition on $\kappa_*(\cdot, \cdot)$ (\Longrightarrow) OK

inf-sup condition on $a(\cdot, \cdot)$ on the kernels of $\kappa(\cdot, \cdot)$ and $\kappa_*(\cdot, \cdot)$ (\Longrightarrow) ??

 $R = R_* \iff$ Things happens exactly as for ψ - ω (Symmetry).

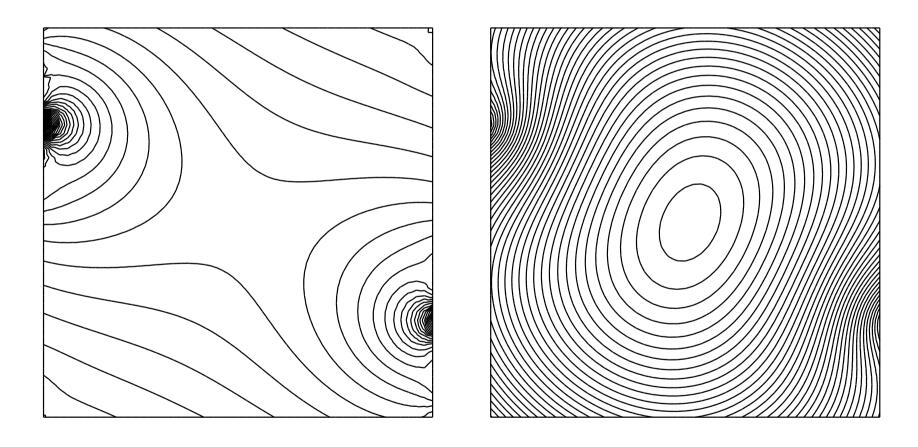
 $R \neq R_*$ (\Longrightarrow) High technical difficulties (only partially solved!)

$$(\Longrightarrow)$$
 osc $(\sqrt{\frac{R}{R_*}}) = \max\sqrt{\frac{R}{R_*}} - \min\sqrt{\frac{R}{R_*}} < 2 ???!!!!,$

 (\Longrightarrow) The constant blows up for small h.

VARIATIONAL FORM IN FREEFEM

FREEFEM



Concentrations b (corrupted) and c.

STABILIZED MFE $\mathcal{P}_1 \times \mathcal{P}_1$

Find b_h and c_h such that

$$\int_{\Omega} (D\nabla b_{h} \nabla \psi_{h} + R b_{h} \psi_{h}) dx = \int_{\Omega} f \psi_{h} dx, \qquad \forall \psi_{h}$$

$$\int_{\Omega} (D\nabla \varphi_{h} \nabla c_{h} + R_{*} \varphi_{h} c_{h}) dx + a_{\rho}(b_{h}, \varphi_{h}) = \int_{\Omega} g \varphi_{h} dx, \qquad \forall \varphi_{h}$$

'Abstract form'

$$\kappa (\psi_h, b_h) = (f, \psi_h), \qquad \forall \psi_h,$$

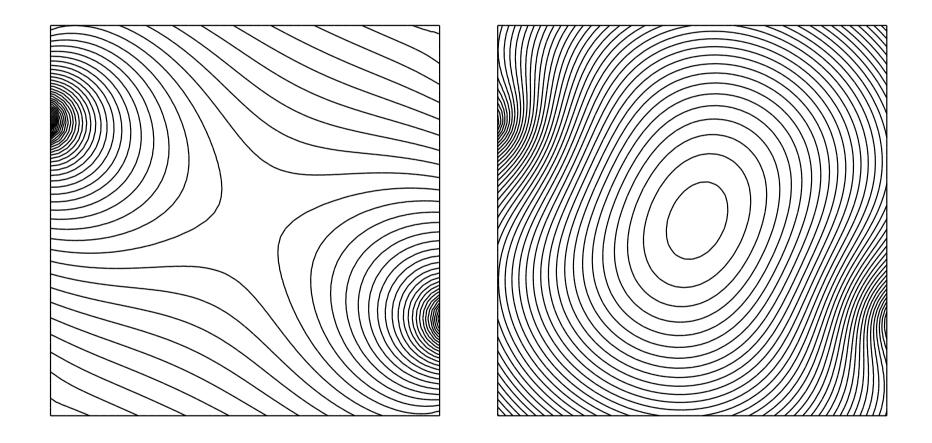
$$\kappa_*(c_h, \varphi_h) + a_{\rho}(b_h, \varphi_h) = (g, \varphi_h), \qquad \forall \varphi_h$$

Stabilization (Amara-Dabaghi, M2AN 2001) —Constant blows up for small h—

$$a_{\rho}(b_h, \varphi_h) = a(b_h, \varphi_h) + \rho \sum_{e \not\subset \partial \Omega} h_e \int_e [D\partial_n b_h]_e(\tau) [D\partial_n \varphi_h]_e(\tau) d\tau.$$

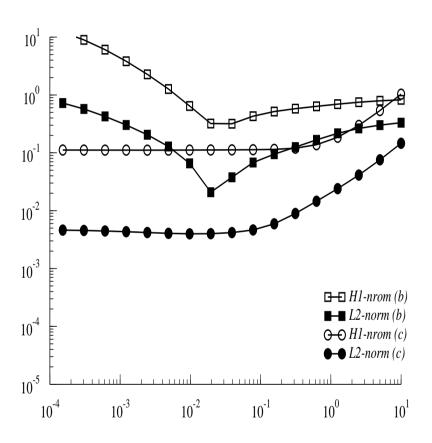
STABILIZATION IN FREEFEM

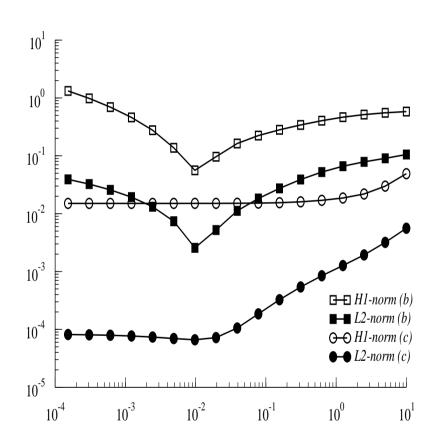
FREEFEM



Concentrations b (corrected by stabilization) and c.

REGULARISATION PARAMETER

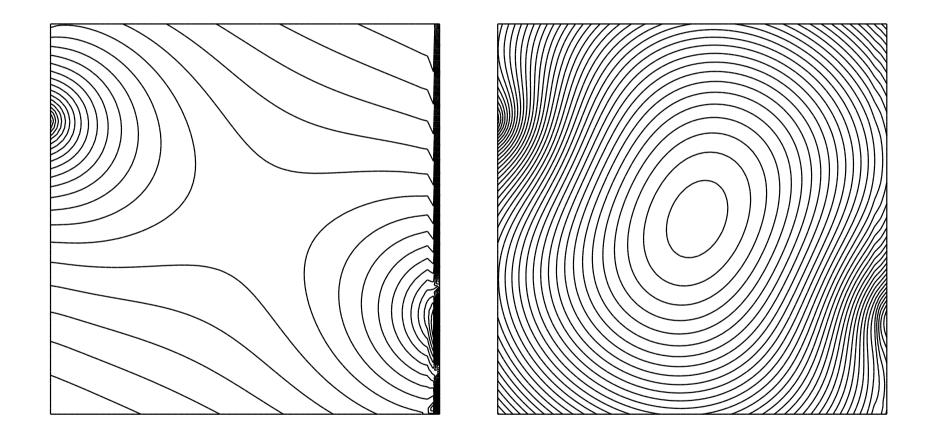




Mesh size h = 1/16 and h = 1/128.

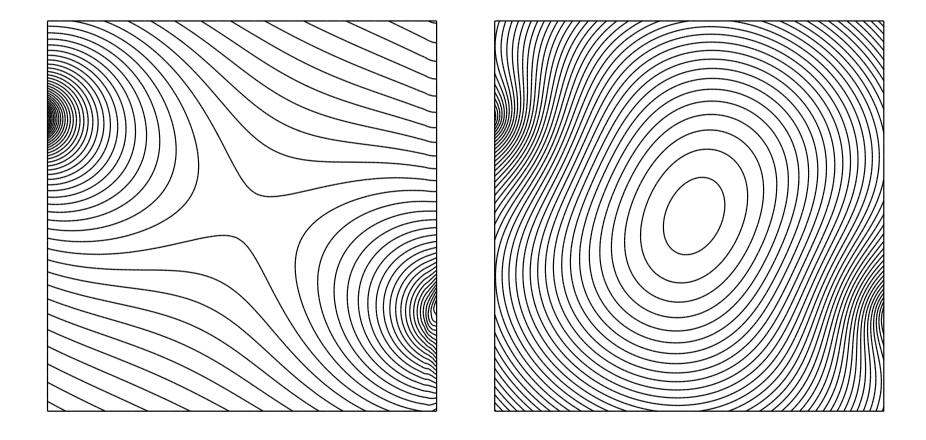
Choice of the parameter $\rho \implies$ Not that Clear?

WITH ADVECTION



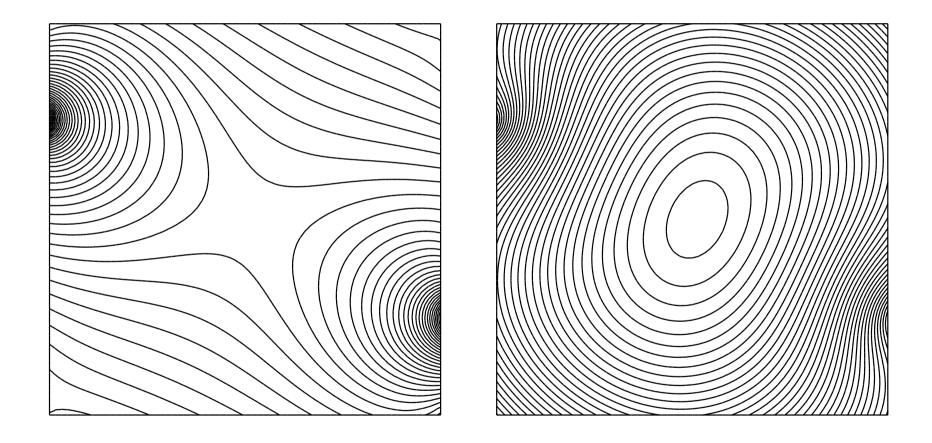
Without stablization.

WITH ADVECTION



With stablization.

Example, osc
$$(\sqrt{\frac{R}{R_*}}) > 13$$



Satabilized Concentrations b and c.

Numerics : (Un)Steady Model

Ben B., Débit, El Fekih, Khiari, (MATLAB)
Journal of Inverse and Ill-posed Problems, <u>In revision</u>.

Azaïez, Ben B., Hecht, Le Bot, (FREEFEM) Inverse Problems, (2014) 30 015002

SPACE DISCRETIZATION

Find $b_h(t)$ and $c_h(t)$ such that : $c_h = 0$ on $\partial \Omega$ and

$$\int_{\Omega} \partial_{t} b_{h}(t) \psi_{h} + \int_{\Omega} (D \nabla b_{h}(t) \nabla \psi_{h} + R b_{h}(t) \psi_{h}) = \int_{\Omega} f(t) \psi_{h},$$

$$\int_{\Omega} \varphi_{h} \partial_{t} c_{h}(t) + \int_{\Omega} (D \nabla \varphi_{h} \nabla c_{h}(t) + R_{*} \varphi_{h} c_{h}(t)) + \int_{\Omega} R b_{h}(t) \varphi_{h} = \int_{\Omega} g(t) \varphi_{h},$$

$$b_{h}(0) = 0, \qquad c_{h}(0) = c_{S}.$$

'Abstract form'

$$(\partial_t b_h(t), \psi_h) + \kappa \left(\psi_h(t), b_h\right) = (f(t), \psi_h), \qquad \forall \psi_h \quad (c_h),$$

$$(\partial_t c_h(t), \varphi_h) + \kappa_* (c_h(t), \varphi_h) + \frac{a_\rho(b_h(t), \varphi_h)}{c_h(0)} = (g(t), \varphi_h), \qquad \forall \varphi_h \quad (b_h),$$

$$b_h(0) = 0, \qquad c_h(0) = c_S.$$

EULER TIME SCHEME (I)

Vectors \boldsymbol{b} and \boldsymbol{c} of Degrees of Freedom. Set $\boldsymbol{Y}^T = (\boldsymbol{b}, \boldsymbol{c})$.

$$\mathbf{M} \mathbf{Y}'(t) + \mathbf{K} \mathbf{Y}(t) = \mathbf{G}(t), \quad \text{in } (0, T)$$

$$\mathbf{Y}(0) = \mathbf{Y}_0.$$

Crude Euler time scheme (τ : time step)

$$egin{aligned} oldsymbol{M}rac{oldsymbol{Y}^{p+1}-oldsymbol{Y}^p}{ au}+oldsymbol{K}oldsymbol{Y}^{p+1}=oldsymbol{G}^{p+1},\ oldsymbol{Y}^0=oldsymbol{Y}_0. \end{aligned}$$

Is the induction well defined?

EULER TIME SCHEME (II)

Setting $\lambda = \tau^{-1}$, we obtain the full discrete problem

$$(\lambda M + K) \mathbf{Y}^{p+1} = G^{p+1} + \lambda M \mathbf{Y}^{p},$$

 $\mathbf{Y}^{0} = \mathbf{Y}_{0}.$

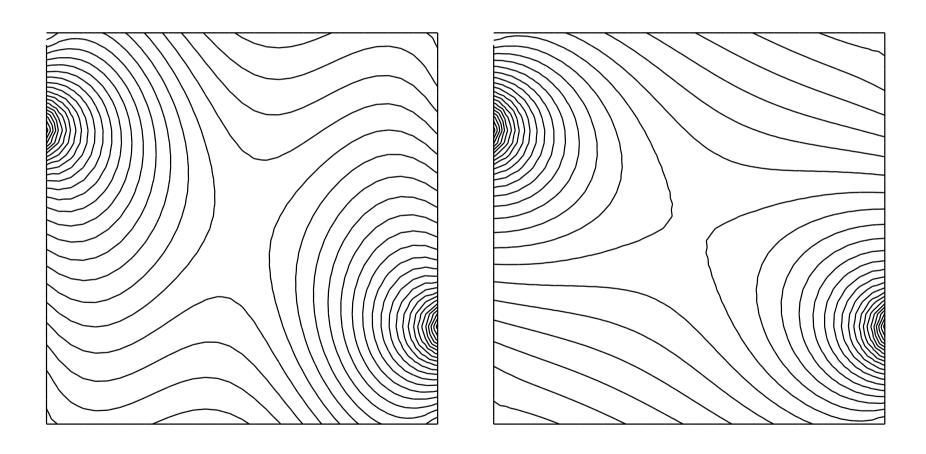
$$(\Longrightarrow)$$
 Is $(\lambda M + K)$ invertible?

 (\Longrightarrow) Look at the mixed problem with $R:=R+\lambda$ and $R_*:=R_*+\lambda$.

$$(\Longrightarrow)$$
 osc $(\sqrt{\frac{R}{R_*}}) = \max \sqrt{\frac{R}{R_*}} - \min \sqrt{\frac{R}{R_*}} < 2.$, EASY !!! FAAACILE!

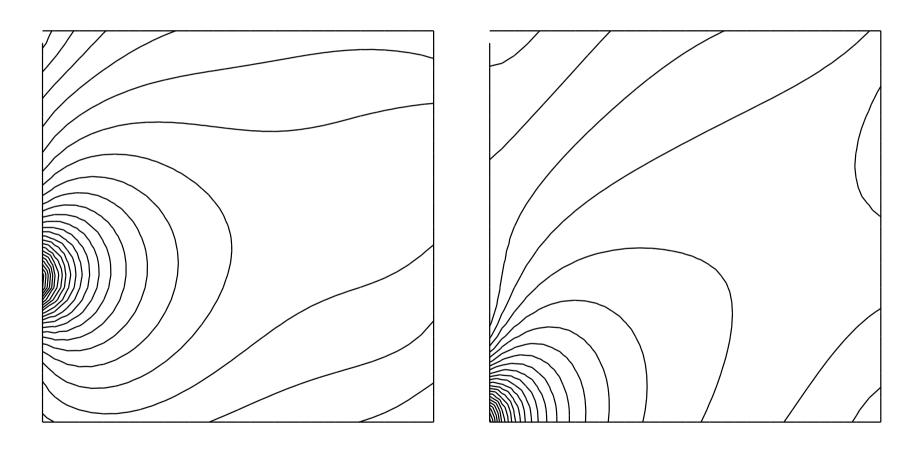
Prop. 2 The discrete problem has a unique solution.

FREEFEM (EXACT DATA)



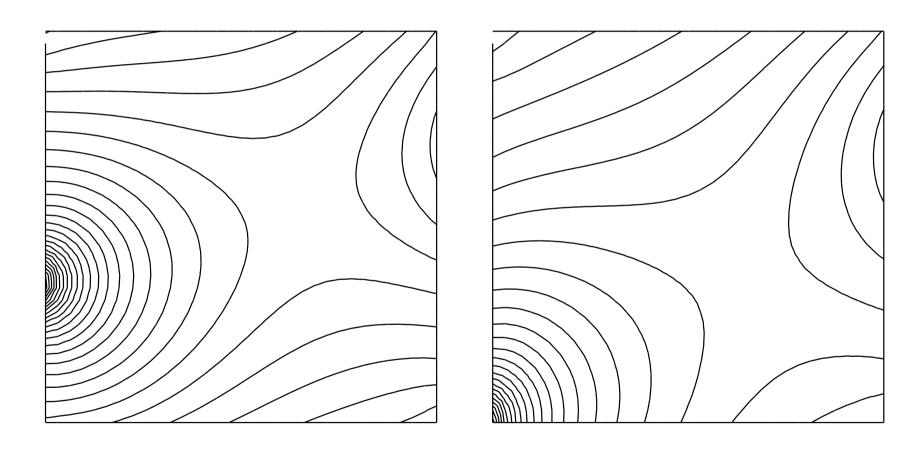
Steady solutions (b, c), t = 1.25 and t = 2.5).

FREEFEM (EXACT DATA)



Unsteady solutions (b, c), t = 0.25 and t = 0.5.

FREEFEM



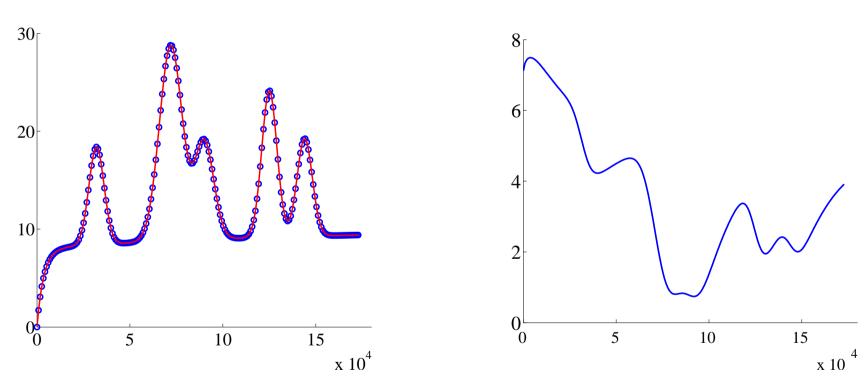
Unsteady solutions (ω, ψ) , t = 0.25 and t = 0.5.

QUANTITATIVE COMPARISON

	H^1	L^2	H^1	L^2	L^{∞}	L^{∞}
Oxyg. balance	1.533 (b)	0.040 (b)	0.478 (c)	0.017 (c)	1.022 (b)	0.012 (c)
Fluid Flow	$0.197 (\omega)$	$0.037 (\omega)$	$0.028 \; (\psi)$	$0.002 \; (\psi)$	$0.112 (\omega)$	$0.002 \; (\psi)$

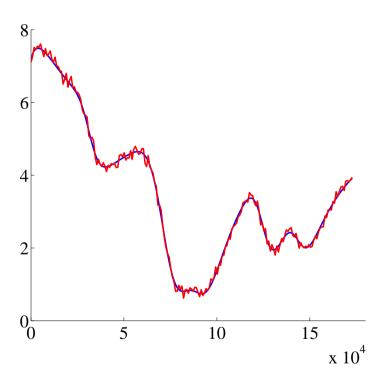
Various relative errors.

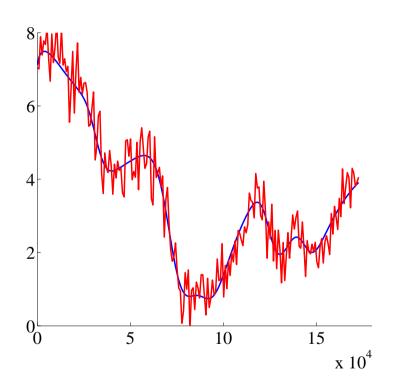
SIMULATIONS 1D (MATLAB)



BOD load b(0,t). Synthetized DO profile $\alpha(t)=c(0,t)$.

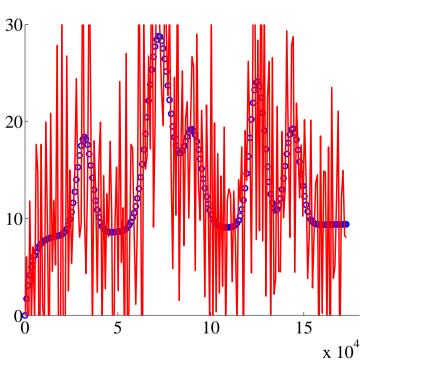
Noisy DO profiles $\alpha(\cdot)$

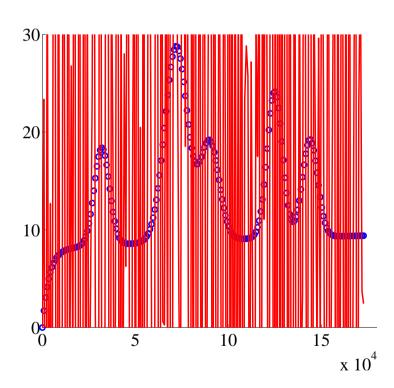




Standard deviation $\sigma = 0.1$ (left) and $\sigma = 0.5$ (right)

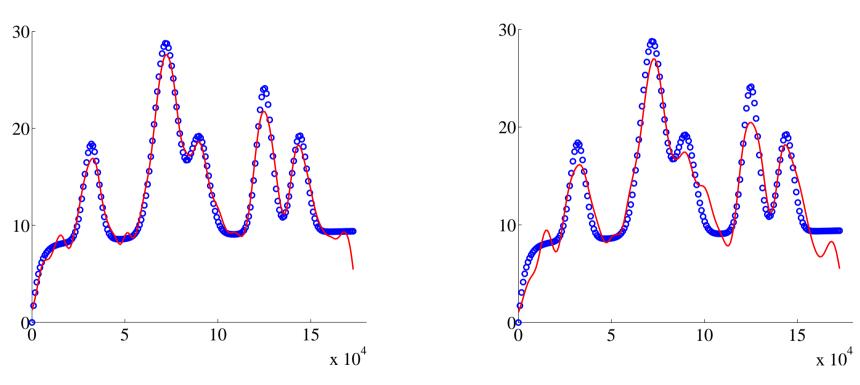
POLLUTED BOD LOADS b(0,t)





 $\sigma = 0.1$ —left— and $\sigma = 0.5$ —right—

FILTERED BOD LOADS b(0,t)



Gaussian Filter, $\sigma=0.1$ —left— and $\sigma=0.5$ —right—

Back to the Semi-Discrete Problem

Vectors **b** and **c** of Degrees of Freedom (\iff) FE functions b_h and c_h .

$$\dim \mathbf{b} = \mathbf{p} = DOF(\Omega), \qquad \dim \mathbf{c} = \mathbf{q} = DOF(\Omega \setminus \partial \Omega)$$

The discrete problem can be expressed as a block linear system

$$\begin{pmatrix} M & 0 \\ 0 & M^T \end{pmatrix} \partial_t \begin{pmatrix} \mathbf{b}(t) \\ \mathbf{c}(t) \end{pmatrix} + \begin{pmatrix} K & 0 \\ A_{\rho} & K_*^T \end{pmatrix} \begin{pmatrix} \mathbf{b}(t) \\ \mathbf{c}(t) \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ \mathbf{g}(+)\boldsymbol{\alpha}(t) \end{pmatrix}, \quad \text{in } (0, T).$$

Set $\mathbf{Y}^T = (\mathbf{b}, \mathbf{c})$. Then the following condensed form

$$\mathbf{M} \mathbf{Y}'(t) + \mathbf{M} \mathbf{Y}(t) = \mathbf{G}(t), \quad \text{in } (0, T)$$

$$\mathbf{Y}(0) = \mathbf{Y}_0.$$

Looks like a differential equation. But ... It is not!

Why it is not?

 $\dim \mathcal{N}(\mathbf{M}) = (p-q)$. Then \mathbf{M} is singular. Prop. 3

Take $Y \in \mathcal{N}(M) \iff (b_h, c_h) : \text{F.E. functions.}$ WHY?

The following orthogonalities hold: $b_h(p)$, $c_h(q)$, $p-q=DOF(\partial\Omega)$

$$\int_{\Omega} b_h \psi_h \, dx = 0, \qquad \forall \psi_h(q),$$

$$\int_{\Omega} c_h \varphi_h \, dx = 0, \qquad \forall \varphi_h(p).$$

$$\int_{\Omega} c_h \varphi_h \ dx = 0, \qquad \forall \varphi_h(p).$$

 $(\Longrightarrow) c_h = 0.$

 (\Longrightarrow) $b_{h|\partial\Omega}$ fully specifies b_h (\Longrightarrow) (p-q) $(DOF) = \dim \mathcal{N}(M)$.

Kronecker Weierstrass canonical form

Problem in Y is an <u>IMPLICIT</u> differential algebraic equation — <u>DAE</u>—.

Important! Uncouple the DE from the AE.

Prop. 4 There exist $LY = (u, v)^T$ and $HG = (q, r)^T$ such that

$$\begin{pmatrix} I_{(2q)} & 0 \\ 0 & N \end{pmatrix} \partial_t \begin{pmatrix} \boldsymbol{u}(t) \\ \boldsymbol{v}(t) \end{pmatrix} + \begin{pmatrix} W & 0 \\ 0 & I_{(p-q)} \end{pmatrix} \begin{pmatrix} \boldsymbol{u}(t) \\ \boldsymbol{v}(t) \end{pmatrix} = \begin{pmatrix} \boldsymbol{q}(t) \\ \boldsymbol{r}(t) \end{pmatrix}.$$

u: differential variable.

v: algebraic variable.

N: square of dimension (p-q). It is nilpotent of order μ .

W: square matrix of dimension (2q).

Uncoupling |

Solve the ordinary differential problem

$$\partial_t \mathbf{u}(t) + W \mathbf{u}(t) = \mathbf{q}(t)$$
 in $(0, T)$,
 $\mathbf{u}(0) = \mathbf{u}_0$,

Unique solution

$$u(t) = e^{-Wt}u_0 + \int_0^t e^{-W(t-s)}q(s) ds.$$

Solve the algebraic equation

$$N\partial_t \mathbf{v}(t) + \mathbf{v}(t) = \mathbf{r}(t)$$
 in $(0, T)$, $\mathbf{v}(0) = \mathbf{v}_0$.

Hypothetic solution

$$\mathbf{v}(t) = \sum_{j \le \mu - 1} (-1)^j N^j \mathbf{r}^{(j)}(t) \iff \sum_{j \le \mu - 1} (-1)^j N^j \mathbf{r}^{(j)}(0) = \mathbf{v}_0.$$

EXISTENCE AN UNIQUENESS

Prop. 5 The semi-discrete problem has at most one solution.

REM. 1 Existence is guaranteed only for consistent initial data $(\boldsymbol{b}_0, \boldsymbol{c}_0)$ and the boundary condition $\boldsymbol{\alpha}$

Kronecker index, Time Scheme

Prop. 6 The Kronecker index is one, $\mu = 1$. As a consequence, N = 0.

Rem. 2 Euler should be sufficient (\Longrightarrow) Yes! May be and may be NO!

CONCLUSION

A lot of computational work is waiting!

PERSPECTIVE

Achieve that work!

Point source detection.