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Numerical techniques for stiff and multiscale differential equations

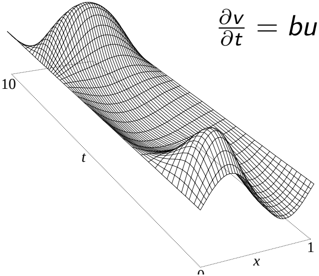
Assyr Abdulle - Mathematics Section
Swiss Federal Institute of Technology, Lausanne (EPFL)

Outline:

1) Methods based on stability

2) Methods based on averaging and homogenization

Ex.: A chemical reaction (the Brusselator) *(Prigogine, Lefever, Nicolis ∼ 1970)*

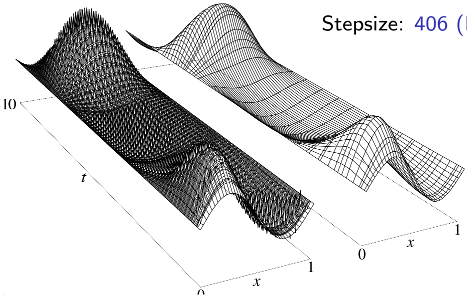


$$\frac{\partial u}{\partial t} = a + u^2 v - (b+1)u + \alpha \triangle u + f(x_1, \ldots, x_d, t)$$
$$\frac{\partial v}{\partial t} = bu - u^2 v + \alpha \triangle v$$

Parabolic PDEs $\Rightarrow$ MOL $\Rightarrow$ ODEs in $\mathbb{R}^{2N^d}$ $\left(\Delta x = \frac{1}{N+1}\right)$

Multiple time scales (Stiffness). Eigenvalues of Jacobian: $\lambda_i \in [-\mathcal{O}(N^2), 0]$

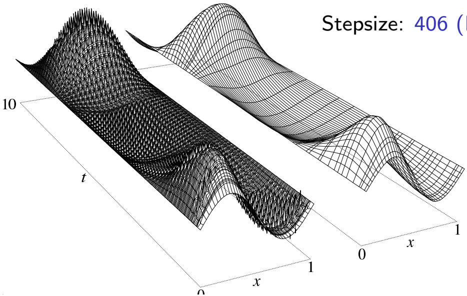
DOPRI5 (Trad. explicit solver) ROCK



Stepsize: 406 (DOPRI5), 16-39 (ROCK4-ROCK2)

DOPRI5
(Trad. explicit solver)

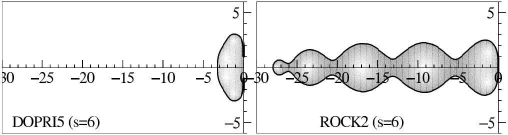
ROCK



Stepsize: 406 (DOPRI5), 16-39 (ROCK4-ROCK2)

Stepsize restriction for trad. explicite solver: $\Delta t \leq C(\Delta x)^2 = C\frac{1}{(N+1)^2}$

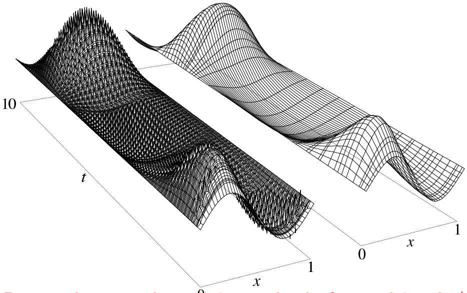
Stability domains: $Y_{n+1} = R(\Delta t J)Y_n, \qquad \Delta t\lambda \in S = \{z \in \mathbb{C}; |R(z)| \leq 1\}$



Based on stability: fcn eval. M fcn. eval $C\sqrt{M}$

ROCK: a stiff (multiscale) solver *A.A. and Medovikov Numer. Math. 01, A.A SIAM SISC. 02, A.A. DCDS 05*

DOPRI5 ROCK
(Trad. explicit solver)



Research around explicit methods for multiscale/stiff problems

Chebyshev methods

...

van der Houwen, Shampine, Sommeijer, Verwer (RKC, IMEX 80-2007)

Bogatyrev, Lebedev, Skvorstov, Medovikov (DUMKA 76-2004)

A.A, Medovikov (ROCK 00-02), A.A. (ROCK 02-05)

A.A, Cirilli, Li, Hu (S-ROCK 07-09,τ-ROCK methods 09)

Projective methods

Gear, Kevrekidis , Lee (projective methods 03-09)

Eriksson, Johnson, Logg (multi-adaptive stabilized methods 03-06)

Heterogeneous Multiscale Methods (ODEs, SDEs)

E, Engquist, Vanden-Eijnden, Tsai, ... 03-09)

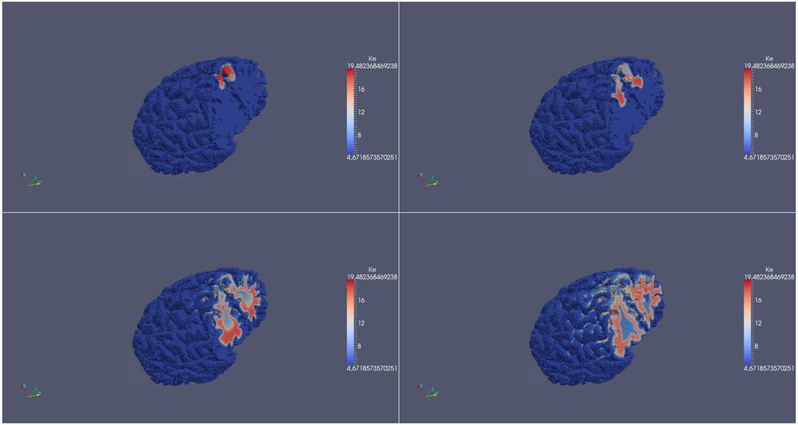
...

Application: Simulation of a Stroke *S. Descombes, T. Dumont, M.-A. Dronne, E. Grenier 2009*

System of 19 react.-diffus. equations $\frac{du_i}{dt} = \alpha_i \triangle u_i + f_i(u_1, \cdots, u_{19})$

Very stiff. Unknowns: ions, volume neurons/non-neurons cells, membrane potentials.

Stroke: change of ions distribution triggers brain cells necrosis



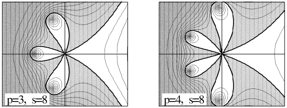
Numerical solution: Strang-Marchuk splitting (RDR)

ROCK4 (explicit, diffusion), RADAU5 (implicit, reactions).

1) Characterization of optimal stability polynomials:

$R_s^p(x) = 1 + x + x^2/2 + .. + x^p/p! + \sum_{j=p+1}^{s} \alpha_j x^j$,

bounded by 1 in largest interval $[-l_s^p, 0]$. Crucial: $l_s^p \propto s^2$.



$A = \{z \in \mathbb{C}; |R_s^p(z)| > |e^z|\}$

Theorem. $R_s^p(x) = w_p(x) P_{s-p}(x)$, $(w_p(x) > 0$, p even)

(using order stars introduced by Wanner, Hairer, Norsett 78)

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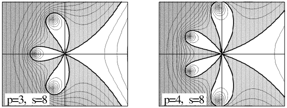

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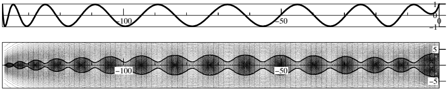
2) Approximation based on orthogonal polynomials (inspired by Bernstein (1930))

$R_s^p(z) \sim \widetilde{w}_p(z) \widetilde{P}_{s-p}(z)$, $\widetilde{P}_{s-p}(z)$ orthog. w.r. $\frac{\widetilde{w}_p(z)^2}{\sqrt{1-z^2}}$ (recursion formula).



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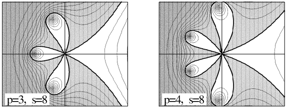

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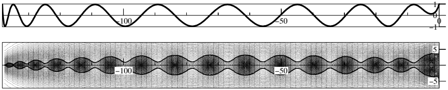

3) Construction of Runge-Kutta (RK) method using **Butcher group**:

Compose RK methods $W(s,p) \circ P(s,p) =: C(s,p)$

$\Rightarrow$ high order methods with variable stages

- explicit methods (no linear algebra problems);
- easy to implement;
- extended stability domains (along $\mathbb{R}^-$);
- low memory demand (recursion formula);
- adaptive in stage number (stability) and stepsize (accuracy).

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Recent developments: **Chebyshev methods for stochastic problems.**

S-ROCK for stiff SDEs A.A. and Cirilli, C.R. Acad. Sci. 07, SIAM SISC 08, A.A. and Li, Comm. Math. Sci. 08.

$\tau-$ROCK for problems with discrete noise A.A., Y. Hu and T. Li, J. Comput. Math. 09 to appear.

Non-trivial extension of ROCK methods:

$\Rightarrow$ extended mean-square stability, approximation by orthogonal polynomials, variable stages, various type of noise.

Analysis:

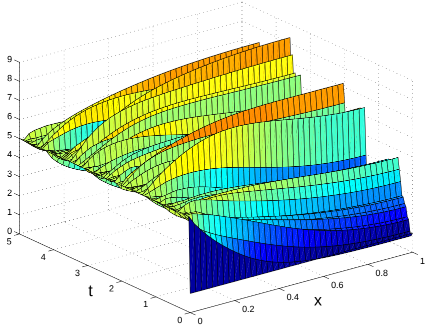
Weak and strong convergence results.

$$\frac{\partial u}{\partial t}(t,x) = D\frac{\partial^2 u}{\partial x^2}(t,x) + ku(t,x)\dot{W}(t)$$

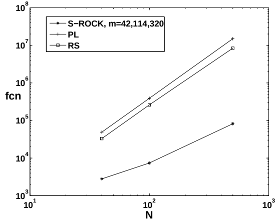
Parameters: $D = 1$, $k = 1$, $u(0,x) = 1$, Mixed boundary conditions $u(t,0) = 5$, $\frac{\partial u(t,x)}{\partial x}|_{x=1} = 0$.

Space discretization.

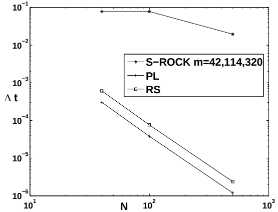
$$dY_t^i = \frac{Y_t^{i+1} - 2Y_t^i + Y_t^{i-1}}{(\Delta x)^2}dt + Y_t^i\ dW_t,\ \ i = 1,\dots,N$$



Ex.:Heat equation with noise (SPDE) solved by S-ROCK method



Function evaluations for the stable integration (strong error $< 10^{-1}$)



Stepsize for the stable integration

Other examples.

Propagation of electrical potential in a neuron (space-time white noise) $S-$ROCK method.

Stiff chemical reactions: "Chemical Langevin Equation" model $\Rightarrow$ $S-$ROCK method,
"Poisson jump process" model $\Rightarrow$ $\tau-$ROCK method.

Example (non mean-square stable problem).

$$dX = f(X,Y)dt$$
$$dY = \frac{1}{\varepsilon}g(X,Y)dt + \frac{1}{\sqrt{\varepsilon}}\sigma(X,Y)dW_t$$

Effective dynamics: $d\bar{X} = \lim_{\varepsilon\to 0}\int f(\bar{X},Y)d\mu^{\varepsilon}_{\bar{X}}(dy) = F(\bar{X})$

Methods based on stability concepts (as S-ROCK or implicit methods):
may not capture the right invariant measure for non mean-square stable problems (damping of the fast scales).

Remedy ⇒ methods based on averaging or homogenization:
estimate numerically the effective forces (e.g. $F(\bar{X})$)

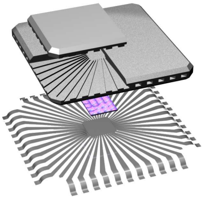
(see Vanden-Eijnden Comm. Math. Sci. 03; E, Liu, Vanden-Eijnden Comm. Pure Appl. Math. 05).

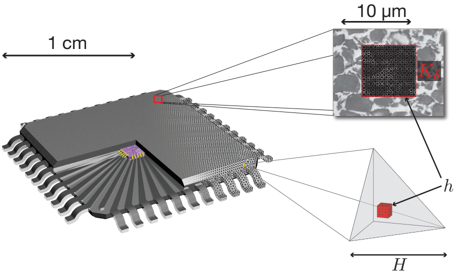
Outline:

I) Methods based on stability

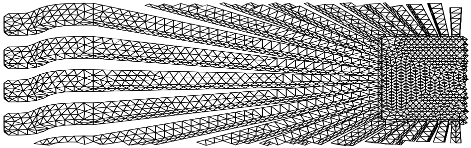
2) Methods based on averaging and homogenization

Ex1: Heat distribution in microprocessor *(A.A and Nonnenmacher CMAME 09)*





Size of processor: $12 \times 12 \times 1$ mm^3, Macro-mesh 430 000 tetrahedras.
3 components, 3 tensors: $a^{\varepsilon}_{lf}(x), a^{\varepsilon}_{pack}(x), a_{chip}(x)$.
Robin boundary conditions (heat exchange with surrounding), heat source: chip work.



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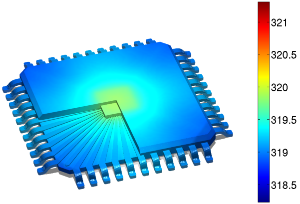
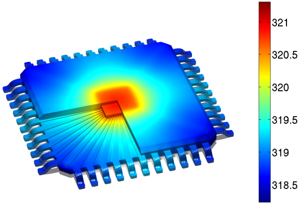
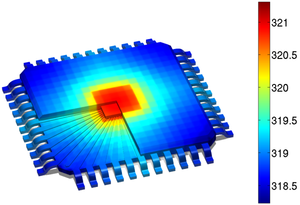
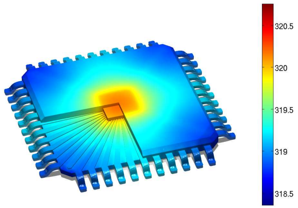
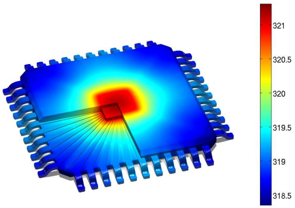






Microstructure : $\sim 5 \cdot 10^{-5}$
FEM (unresolved DOF: $\sim 8 \cdot 10^4$), FE-HMM (Macro DOF: $8 \cdot 10^4$).
Fine scale (DOF: $\sim 4 \cdot 10^6$, $\sim 2.2 \cdot 10^7$ tetrahedras).





Microstructure : $\sim 10^{-6}$
FE-HMM $\sim 8 \cdot 10^4$ Macro DOF, two different micro resolutions.
Fine scale: would need at least 10^{11} DOF.

Remark. Domain decomposition type multiscale methods (solving fine scales on whole triangles): at least $8 \cdot 10^4 \cdot 10^6$ DOF !

Macro-to-micro multiscale method (HMM) *(E, Engquist Comm. Math. Sci. 2003)*

Multiscale problem: $L^{\varepsilon}(u^{\varepsilon}, D^{\varepsilon}) = f$ in $V(\Omega)$

Effective problem: $L^{0}(u^{0}, D^{0}) = f$ in $V(\Omega)$, D^{0} unknown

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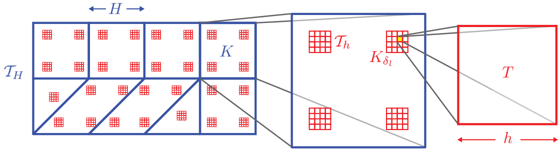
Effective problem: $L^0(u^0, D^0) = f$ in $V(\Omega)$, D^0 unknown

Consider a macro discretization: $\bigcup_{K\in\mathcal{T}_H} K = \Omega$ $\quad H = \text{diameter}(K) >> \varepsilon$

Heterogeneous Multiscale Methods (HMM):

- Macro method: Define $L_H(u^H) = f$ in $V_H(\Omega, \mathcal{T}_H)$ (L_H unknown).
- Micro method: $u^h - u^H \in S_h(K_\delta, \mathcal{T}_h)$ recover L_H by micro sampling

$$L_H(u^H)|_K \sim L_h^\varepsilon(u^h, D^\varepsilon)|_{K_\delta} \quad K_\delta \text{ sampling domain } \subset K$$



Example.

a) Multiscale problem: $u^\varepsilon \in H_0^1(\Omega)$ $\int_\Omega a^\varepsilon(x)\nabla u^\varepsilon \cdot \nabla v dx = \int_\Omega f v dx, \ \forall v \in H_0^1(\Omega)$

b) Effective problem: $u^0 \in H_0^1(\Omega)$ $\int_\Omega a^0(x)\nabla u^0 \cdot \nabla v dx = \int_\Omega f v dx, \ \forall v \in H_0^1(\Omega)$

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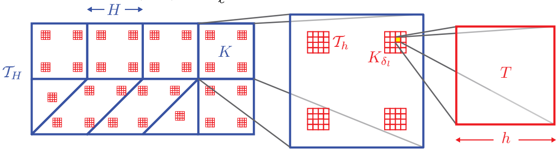
1) Macro discretization. $v^H, w^H \in V_H^p(\Omega, \mathcal{T}_H), \quad H >> \varepsilon$

$$B(v^H, w^H) := \sum_{K\in\mathcal{T}_H} \sum_{\ell=1}^{L} \frac{\omega_{K_\ell}}{|K_\delta|} \int_{K_{\delta_\ell}} a^\varepsilon(x) \nabla v_\ell^h \cdot \nabla w_\ell^h dx$$



2) Microscopic sampling. v_ℓ^h (resp. w_ℓ^h) minimize an energy

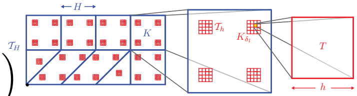
$$v_\ell^h = \text{argmin}_{(\eta^h - v^H)\in S_h^q(K_{\delta_\ell}, \mathcal{T}_h)} \int_{K_{\delta_\ell}} a^\varepsilon(x)\nabla \eta^h \cdot \nabla \eta^h dx$$

3) Variational problem.

$$B(u^H, w^H) = \int_\Omega f w^H dx \ \ \forall w^H \in V_H(\Omega, \mathcal{T}_H)$$

Examples of a priori estimates:

$$\|u^0 - u^H\|_{H^1(\Omega)} \leq C\left(H^p + \left(\frac{h}{\varepsilon}\right)^{2q} + m_e\right)$$
$$\|u^0 - u^H\|_{L^2(\Omega)} \leq C\left(H^{p+1} + \left(\frac{h}{\varepsilon}\right)^{2q} + m_e\right)$$



Remarks:

- C independent of ε but depend on the upscaled solution u^0;
- estimates for macro- and micromeshes are sharp;
- m_e modeling error, can be estimated in some cases (e.g. $a^\varepsilon(x) = a(x, x/\varepsilon)$ periodic in fast variable $\Rightarrow m_e \equiv 0$);
- $h = \frac{\varepsilon}{(N_{mic})^{1/d}}$, thus $\frac{h}{\varepsilon} = \frac{1}{(N_{mic})^{1/d}}$ independent of ε (N_{mic} micro DOF);
- small scale recovery by extension of microsolution or local problems;
- results and numerics for nonlinear and stochastic problems (E, Ming, Zhang AIMS 05, A.A. Gakuto Intern. Series, Math. Sci. and Appl., 2009);
- residual based a posteriori error estimates (A.A and Nonnenmacher, C.R. Acad. Sci 09).

Recent developments of the FE-HMM

FE-HMM for problems in elasticity (A.A. M3AS 06)
Hybrid coupling for HMM (macro FEM, micro spectral) (A.A and Engquist, SIAM MMS 07)
Discontinuous Galerkin FE-HMM (A.A C.R. Acad. Sci. 07)
FE-HMM code for homogenization problems (A.A and Nonnenmacher, CMAME 09, code available at http://iacs.epfl.ch/anmc)
A posteriori error analysis of HMM for homogenization problems (A.A and Nonnenmacher, C.R. Acad. Sci.09)
HMM for wave equation (A.A and M. Grote 09)

Also for time-dependent PDEs

Multiscale methods for advection diffusion problems (A.A. AIMS DCDS 05)
HMM for parabolic problems (A.A and E, JCP 03, A.A and Nonnenmacher, CMAME 09, Ming, Zhang Math. Comp. 07)

Book to appear: Multiscale Problems in Biomathematics, Physics and Mechanics
(A.A, Damlamian, Banasiak, Sango), *Gakuto Intern. Series, Math. Sci. and Appl., 2009*

Other recent multiscale methods (non exhaustive list !!!)

- (Iterative coupling, represent. volume elements: Kouznetsova, Geers et al.; Terada, Kikuchi; Guedes; Miehe et al.; Fish,Belsky; FE^2 Feyel, Chaboche (95-09))
- (Multigrid Homogenization: Neuss, Jaeger, Wittum (00-05),..)
- (Wavelet-based Homogenization: Beylkin, Brewster; Engquist, Runborg; Daubechies, Runborg, Zou (95-08), ...)
- (Multiscale FEM (modified basis functions): Hou,Wu,Cai, Efendiev, Ginting (99-08); Allaire, Brizzi (05) Residual free bubbles FEM, Sangalli (03), Harmonic coordinates, Owhadi, Zhang (06))
- (Two-scale FEM, Sparse FEM: Matache,Schwab (02),Schwab,Viet Ha Hoang (05),Viet Ha Hoang (09))
- (Adaptive (variational) multiscale methods: Nolen, Papanicolaou, Pironneau 08)
- (Adaptive hierarchical modeling: Oden, Zohdi, Rodin, Vemaganti, Prudhomme, Bauman, Romkes (96-09))