

DE LA RECHERCHE À L'INDUSTRIE



# Acceleration methods for fixed point coupled problems iterations

Coupled Problems 2017 |

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12-14 JUNE 2017

Numerical Methods in Coupled Problems

- **Fixed point iterations acceleration**
- **A generic residual-based acceleration method**
- **Numerical experiments**
- **Conclusions and perspectives**

# Fixed point iterations acceleration

## Fixed point iterations

$$X_{n+1} = F(X_n), \text{ until } \|F(X_n) - X_n\| \leq \varepsilon$$

are still the **most common approach** to dealing with a variety of numerical problems :

- **coupled problems** : partitioning multi-physics, domain decomposition, proper generalized decomposition,...
- **nonlinear problems** : heat transfer, nonlinear mechanics, electronic structure,...

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☹️ : often **slow and poor (linear) convergence**

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↔ **acceleration methods** (aka extrapolation methods) for sequence convergence

$$X_{n+1} = G(F(X_n), F(X_{n-1}), \dots, X_n, X_{n-1}, \dots), \text{ until } \|F(X_n) - X_n\| \leq \varepsilon$$

which aim to **converge faster** (in less iterations and computational cost) to the solution  $\bar{X}$ .

- Most popular and efficient acceleration method for first order sequences remains **the  $\Delta^2$  of Aitken** (1926) :

### Aitken $\Delta^2$ -method (static sequence transformation)

Assuming  $x_{n+1} - \bar{x} = (\lambda + \varepsilon_n)(x_n - \bar{x})$ ,  $\lim_{n \rightarrow \infty} \varepsilon_n = 0$

Then  $y_n = x_n - \frac{(\Delta x_n)^2}{\Delta^2 x_n}$  with  $\begin{cases} \Delta x_n &= x_{n+1} - x_n \\ \Delta^2 x_n &= \Delta x_{n+1} - \Delta x_n \end{cases}$

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- Dynamic (/cycling/recursive) sequence transformations based on the  $\Delta^2$ -method

- Steffensen algorithm

$$x_{n+1} = x_n - \frac{(f(x_n) - x_n)^2}{f(f(x_n)) - 2f(x_n) + x_n}$$

- two-steps method
- second-order method
- but efficacy index 1.4
- converges even when the basic fixed point iterations diverge !

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- Dynamic (/cycling/recursive) sequence transformations based on the  $\Delta^2$ -method

- Secant method

$$x_{n+1} = x_n - \frac{(x_n - x_{n-1})(f(x_n) - x_n)}{(f(x_n) - x_n) - (f(x_{n-1}) - x_{n-1})}$$

- also called **dynamic relaxation, Aitken relaxation,...**
- one-step method**
- order :  $(1 + \sqrt{5})/2 \simeq 1.6$**
- efficacy index  $1.6 >$  Steffensen method**

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- Dynamic (/cycling/recursive) sequence transformations based on the  $\Delta^2$ -method
  - Many other generalizations of the Aitken's process :  $\varepsilon$ -algorithm,...

- Correspond to the majority of the problems of interest
- Generalization of scalar transformations to vector transformations are non-unique (convergence properties ?...)
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- Generalization of scalar transformations to vector transformations are non-unique (convergence properties ?...)
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  - Most of them are scalar extension using

$$X^{-1} = \frac{X}{\|X\|^2} \quad \text{or more generally} \quad X^{-1} = \frac{Y}{Y \cdot X}$$

- Steffensen → Irons and Tuck, Lemaréchal, Graves-Morris, A-algorithm, Jennings, Zienkiewicz and Lohner,...
- Secant → many variant of the vector secant method, dynamic relaxation method,...
- $\varepsilon$ -algorithm → vector  $\varepsilon$ -algorithm, topological  $\varepsilon$ -algorithm

- Correspond to the **majority of the problems of interest**
- **Generalization of scalar transformations** to vector transformations **are non-unique** (convergence properties ?...)
- **Extensively studied in the literature** in the 60s and since the 90s.
  - Other ones are **directly dedicated to vector sequences** and often based on a **minimization process** (or projection)
    - Nonlinear hybrid procedure and the associated  $\Delta^k$ -method
    - Anderson method (equivalent to the interface quasi-Newton method),
    - Reduced rank extrapolation method, Minimal Polynomial extrapolation method,...

These methods can generally **reduce** (for special choices of parameters) **in the scalar case to the Aitken  $\Delta^2$  method**.

↪ **Generalization of Aitken's method for vector sequences.**

- Correspond to the **majority of the problems of interest**
  - **Generalization of scalar transformations** to vector transformations **are non-unique** (convergence properties ?...)
  - **Extensively studied in the literature** in the 60s and since the 90s.
- ↔ We propose a **common framework** to **build new vector acceleration** methods and to **recover the most popular and efficient** extrapolation methods

# **A generic residual-based acceleration method**



## ■ A generic formalism for vector sequences

### Residual-based acceleration method

Assuming

- $Y_n = X_n - \sum_{i=1}^M \lambda_n^i Z_n^i, \quad \lim_{n \rightarrow \infty} Z_n^i = 0, \lambda_n^i \in \mathbb{R}$
- $Y_{n+1} = X_{n+1} - \sum_{i=1}^M \lambda_n^i Z_{n+1}^i$

Then the minimization of  $\delta Y_n = Y_{n+1} - Y_n$  gives  $\lambda_n^i$  and an estimation of  $\bar{X}$

$$Y_n = X_n - Z_n (\delta Z_n^T \delta Z_n)^{-1} \delta Z_n^T \delta X_n$$

- Generalization for  $M > 1$  of the nonlinear hybrid procedure
- Very close to the polynomial extrapolation formalism : reduced rank extrapolation method recovered for  $Z_n^i = \delta X_{n+i-1}$
- For  $Z_n^i = \delta X_{n-i}$  : basic idea of Anderson method

# Two classes of dynamic methods

- Iterative acceleration for fixed point iterations :
  - two sequences  $(X_n)_n$  and  $(F(X_n))_n$  are generated
  - two main formalisms of iterative residual-based methods are available
- One-step iterative methods (easily transportable to multi-step methods)

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### Crossed sequences method

- $$Y_n = F(X_{n-1}) - \sum_{i=1}^M \lambda_n^i Z_n^i$$

$$Y_{n+1} = F(X_n) - \sum_{i=1}^M \lambda_n^i Z_{n+1}^i$$

- Focus on the basic fixed point sequence  $(F(X_n))_n$
- Take generally into account  $(X_n)_n$  in the definition of  $Z_n^i$
- For  $Z_n^i = F(X_{n-i}) - X_{n-i}$  and  $M = 1$  : standard vector secant (dynamic relaxation) and Irons-Tuck if two-step method.

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### Alternate sequences method

- $$Y_n = X_n - \sum_{i=1}^M \lambda_n^i Z_n^i$$

$$Y_{n+1} = F(X_n) - \sum_{i=1}^M \lambda_n^i Z_{n+1}^i$$

- $Y_n$  is only concerned by  $(X_n)_n$  whereas  $Y_{n+1}$  depends on  $(F(X_n))_n$
- Then  $\delta Y_n$  is a linear combination of fixed point residual  $(F(X_n) - X_n)$  with the same coefficients than the sequence coefficients.
- For  $Z_n^i = X_{n-i+1} - X_{n-i}$  and  $Z_{n+1}^i = F(X_{n-i+1}) - F(X_{n-i})$  : Anderson method.

# Numerical experiments

- Point-wise solver used to perform nonlinear mechanical behaviour unit testings : MTest (MFront) tool, developed in the PLEIADES platform.
- Solved by a quasi-Newton fixed point equation

### Equilibrium resolution

Let  $X = E|_{t+\Delta t} - E|_t$ , then

solve  $R(X) = \Sigma|_{t+\Delta t}(X, \Delta t, V|_t) - \Sigma|_{t+\Delta t}^{imp} = 0$

using

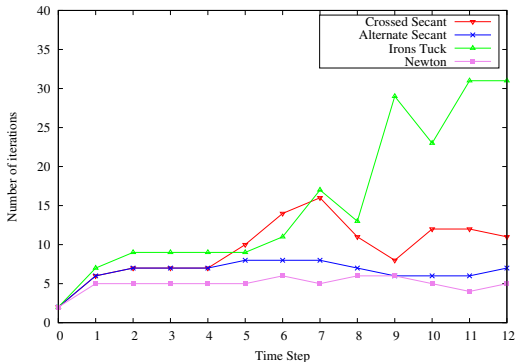
$$X_{n+1} = X_n - H^{-1}R(X_n)$$

with  $H$  : elastic operator

- ☺ :  $H$  easy to compute, symmetrical and definite positive and can be factorized only once (or updated from time to time)
- ☹ : Very slow fixed point linear convergence.

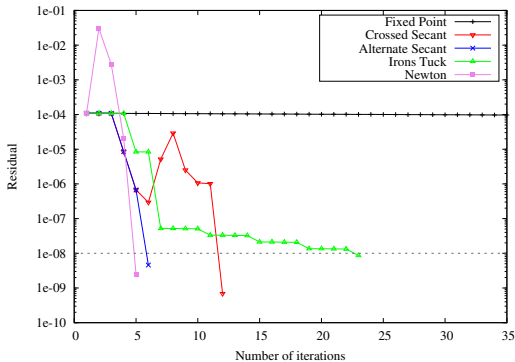
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- Two iteration residual methods comparison + second-order Newton method -  $\varepsilon = 10^{-8}$



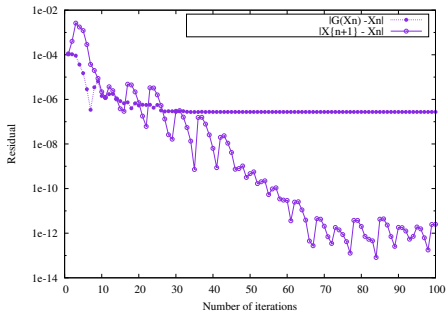


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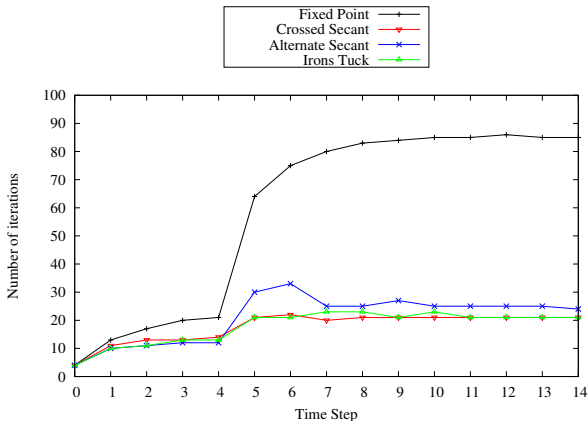
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Crossed 2- $\delta$  method converges but not to the fixed point.

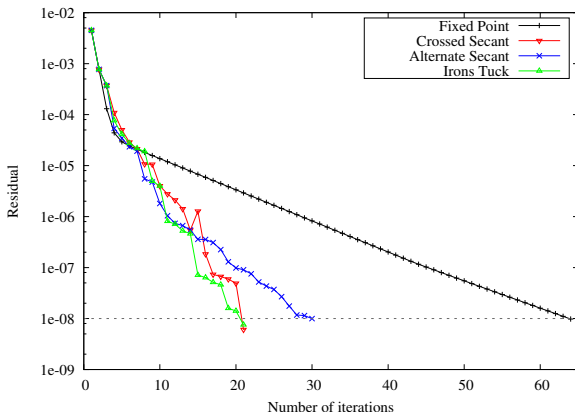


- Fixed point iterations converge faster
- Jacobian matrix unavailable  $\Rightarrow$  no Newton method

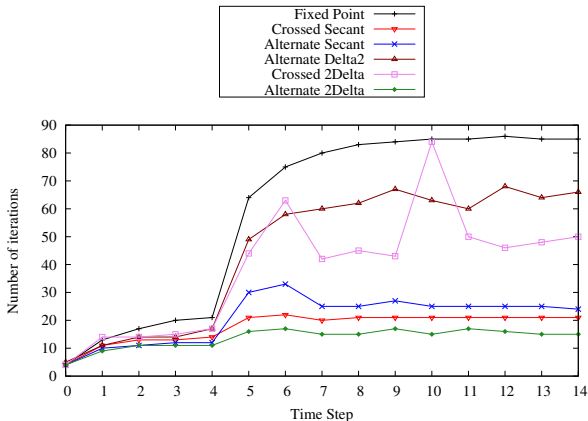
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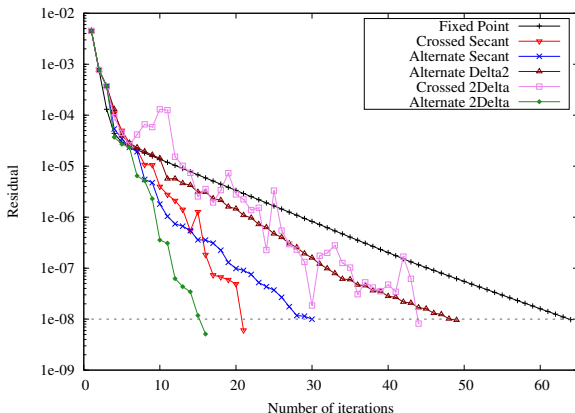
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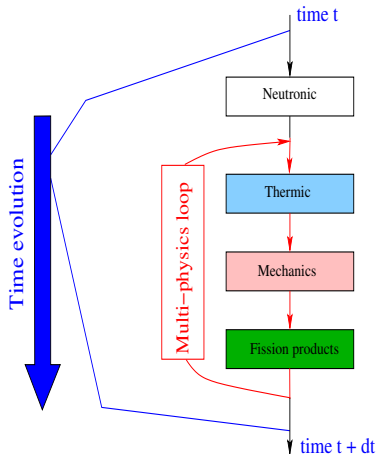


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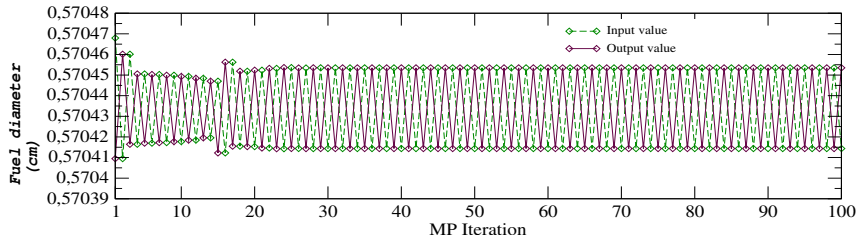


- **Performances** of the acceleration method depend on the test case
- **Secant methods seem really efficient** : they can concurrence the second-order Newton method !
- **Alternate  $M - \delta$  ( $\equiv$  Anderson) methods** seem the best  $M$ -iterates methods.

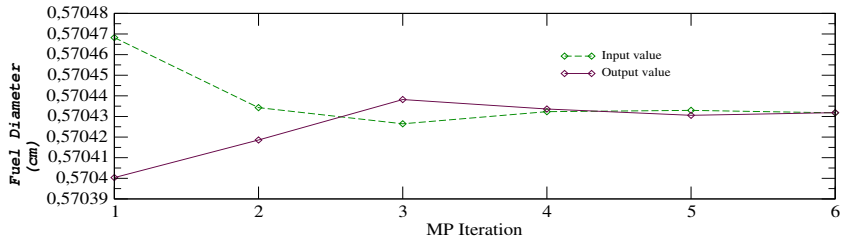


-  platform dedicated to nuclear fuel behaviour simulation
- Partitioning coupling
- Gauss-Seidel multi-physics fixed point iterations

## Fixed point iterations

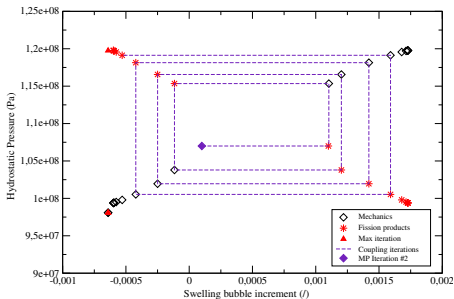


## Crossed secant (dynamic relaxation)

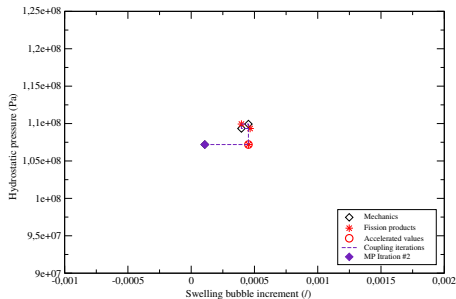


- Crossed secant (dynamic relaxation) not always converge in case of fixed point iterations divergence
- Irons and Tuck method seems always converge but sometimes slower than the fixed point.

Fixed point iterations

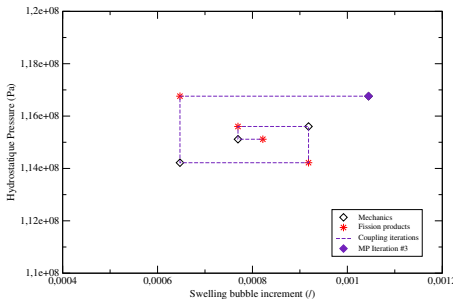


Irons and Tuck acceleration

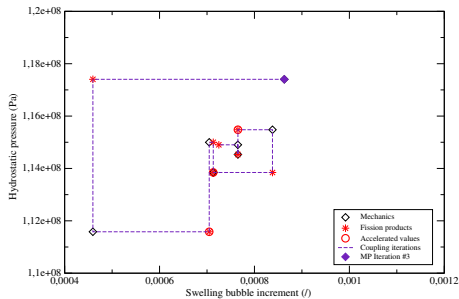


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- Irons and Tuck method seems always converge but sometimes slower than the fixed point.
- Currently trying alternate  $M - \delta$  methods...

# Conclusions

- A **generic residual-based approach** has been introduced to build sequence acceleration processes
  - **generalization** of various existing vector acceleration methods
  - derived in **two main classes of dynamic acceleration methods** :  
crossed and alternate approaches
- A **set of iterative acceleration approaches** have been tested on nonlinear mechanics resolution and multi-physics simulation
  - the **crossed approach is only interesting in its secant**  $(1 - \delta X_n)$  version
  - in particular **alternate  $M - \delta$  (Anderson) approaches** seem the most efficient
- This generic acceleration formalism has **already been successfully applied on other applications** : FFT, PGD,...



# Thank you for your attention

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