Computational Methods for Transient Coupled-Physics Problems
(KAIST Fall 2005/KCP)

18 October 2005: Basic Transient Analysis Techniques

20 October 2005: Staggered Solution Procedures

25 October 2005: Structure-Acoustic Interaction Analysis

27 October 2005: Stabilization Strategies and their Applications

01 November 2005: Fine Points in Transient Analysis Techniques

03 November 2005: Simulation of Multi-Physics Problems

What is stabilization?

Let us consider the following time-discretized difference equation

$$\sum_{k=0}^{m} a_k \mathbf{x}^{m-k} = 0, \tag{1}$$

In lieu of the computational stability discussed in Lecture 01, *stabilization* refers to a strategy to bound the magnitudes of all of the characteristics roots to be less or at most equal unity, that is, for a characteristic equation of the form

$$\sum_{k=0}^{m} a_k \lambda^{m-k} = 0, \quad x^{n+1} = \lambda x^n \tag{2}$$

if the magnitudes of any of its roots exceed unity, stabilization is a mapping that guarantees

$$|\lambda_k| \leq 1, \quad k = 1, 2, \ldots, m. \tag{3}$$

Sources of computational instability

- Use of explicit integration formulas with conditional stability, e.g., $\omega_{max}h \leq 2$ for the case of the central difference formula when applied to integrate undamped structural equations of motion.

- Extrapolation of coupling terms even though each field equations are integrated by unconidtionally stable implicit formulas.

- Use of higher-order implicit integration formulas for accuracy considerations, in violation of G. Dahliquist's A-stability theorem (1963).

Strategies for computational stabilization

- Stabilization by *stiffly A-stable* integration formulas.
- Stabilization via *correctional* steps.
- *Physics-based augmentation* that introduces dissipation into the system without altering the physics of the governing equations of coupled systems.

Stabilization by *stiffly A-stable* **integration**

Consider integrating the undamped structural dynamics equation

$$\mathbf{M}\ddot{\mathbf{x}} + \mathbf{K}\mathbf{x} = f(t) \tag{4}$$

by two different integration formulas:

$$\begin{aligned} &\text{the trapezoidal rule: } \mathbf{x}^{n+1} - \mathbf{x}^{n} - \tfrac{1}{2}h(\dot{\mathbf{x}}^{n+1} + \dot{\mathbf{x}}^{n}) = 0 \\ &\text{the 2-step Gear's formula: } 3\mathbf{x}^{n+1} - 4\mathbf{x}^{n} + \mathbf{x}^{n-1} - 2h\dot{\mathbf{x}}^{n+1} = 0 \end{aligned} \tag{5}$$

The characteristic equations of the integration processes by the two formulas yield:

$$\begin{aligned} &\text{the trapezoidal rule: } |(\lambda - 1)^2\mathbf{M} + \frac{(\lambda + 1)^2}{2}h^2\mathbf{K}| = 0 \\ &\text{the 2-step Gear's formula: } |(3\lambda^2 - 4\lambda + 1)^2\mathbf{M} + (2\lambda)^4h^2\mathbf{K}| = 0 \end{aligned} \tag{6}$$

Projecting the previous characteristic equations onto the modal basis via

$$\mathbf{x} = \mathbf{\Phi q}, \quad \mathbf{\Phi}^T\mathbf{M\Phi} = \mathbf{I}, \quad \mathbf{\Phi}^T\mathbf{K\Phi} = \mathrm{diag}\{\omega_1^2, \omega_2^2, \ldots, \omega_N^2\} \tag{7}$$

we obtain the following modal characteristic equations:

$$\begin{aligned} &\text{the trapezoidal rule: } (\lambda-1)^2 + \frac{(\lambda+1)^2}{2} h^2\omega^2 = 0 \\ &\text{the 2-step Gear's formula: } (\lambda-1)^2(3\lambda-1)^2 + (2\lambda)^2 h^2\omega^2 = 0 \end{aligned} \tag{8}$$

Let us examine two asymptotic limits, viz., the low-frequency limit ($\omega \to 0$) and the high-frequency limit ($\omega \to \infty$).

Low-frequency limit ($\omega \to 0$)*:*

$$\begin{aligned} &\text{the trapezoidal rule: } \lambda_p \to 1 \\ &\text{the 2-step Gear's formula: } \lambda_p \to 1, \quad \lambda_{sp} \to 1/3 \end{aligned} \tag{9}$$

where λ_p is the double principal roots that approximate the solution while λ_{sp} is a spurious root that may hamper the solution accuracy if its magnitude is large. The conclusion is that, when the step size is sufficiently reduced, both formulas can capture the principal solution, i.e., undamped and purely oscillatory response of the modal equation. Specifically, the modal numerical solutions may be expressed as

$$\begin{aligned} &\text{the trapezoidal rule: } q^n = c_1\lambda_{p1}^n + c_2\lambda_{p2}^n \\ &\text{the 2-step Gear's formula: } q^n = d_1\lambda_{p1}^n + d_2\lambda_{p2}^n + d_3\lambda_{sp1}^n + d_4\lambda_{sp2}^n \end{aligned} \tag{10}$$

where the coefficients (c_i, d_i) depend on the initial conditions, and the coefficients (d_3, d_4) turn out to be small so that the contributions of the spurious roots quickly die out.

High-frequency limit ($\omega \to \infty$):

$$\begin{aligned} &\text{the trapezoidal rule:} \quad |\lambda_p| \to 1 \\ &\text{the 2-step Gear's formula:} \quad |\lambda_p| \to 0 \end{aligned} \tag{11}$$

Observe that, in view of the solutions expressed in terms of λ, the trapezoidal rule maintains the contributions of high-frequency components.

On the other hand, the Gear's two-step method dissipates all the high-frequency contributions. As an example, if the trapezoidal rule was used to integrate the acoustic equation instead of the Gear's two-step method, the following stability condition would have resulted in:

$$\begin{aligned} &\text{the trapezoidal rule:} \quad 2-(m-1)\mu h>0, \quad m>1 \\ &\text{the 2-step Gear's formula:} \quad 8-(m-1)\mu h>0, \quad m>1 \end{aligned} \tag{12}$$

Hence, the use of stiffly A-stable algorithm (Gear's two-step method) extends the stability limit of a staggered procedure by four times compared with the trapezoidal rule.

Stabilization via correctional steps

It was shown in the previous lecture that the single-pass staggered procedure leads to conditional stability, which for convenience is reproduced below

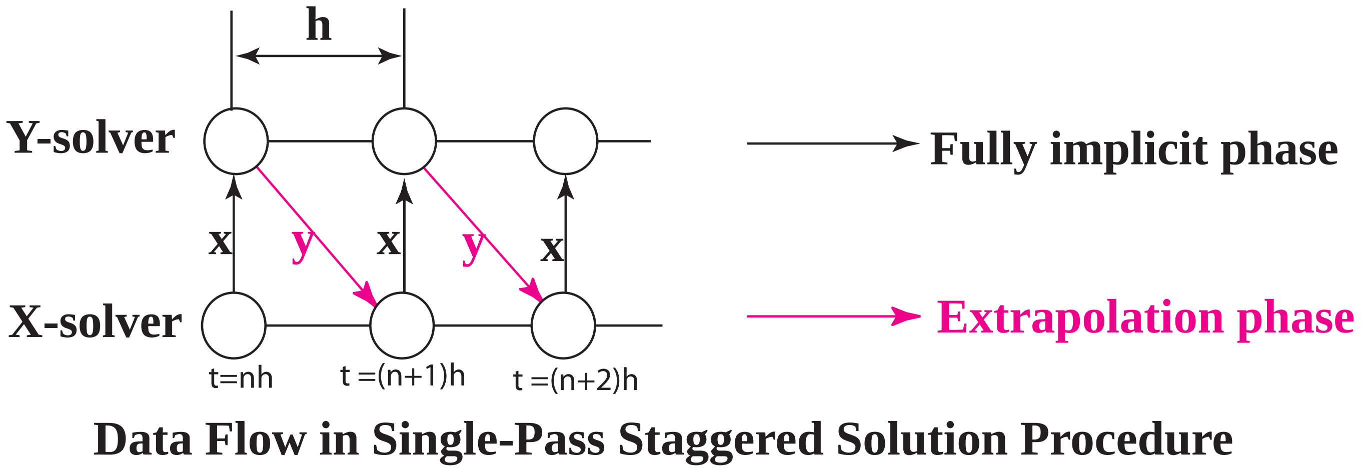

Fig. 1 Single pass staggered algorithm for a tightly coupled problem

In order to extend the stability limit of the single-pass algorithm, one could come up with a double-pass algorithm as shown in Fig. 2.

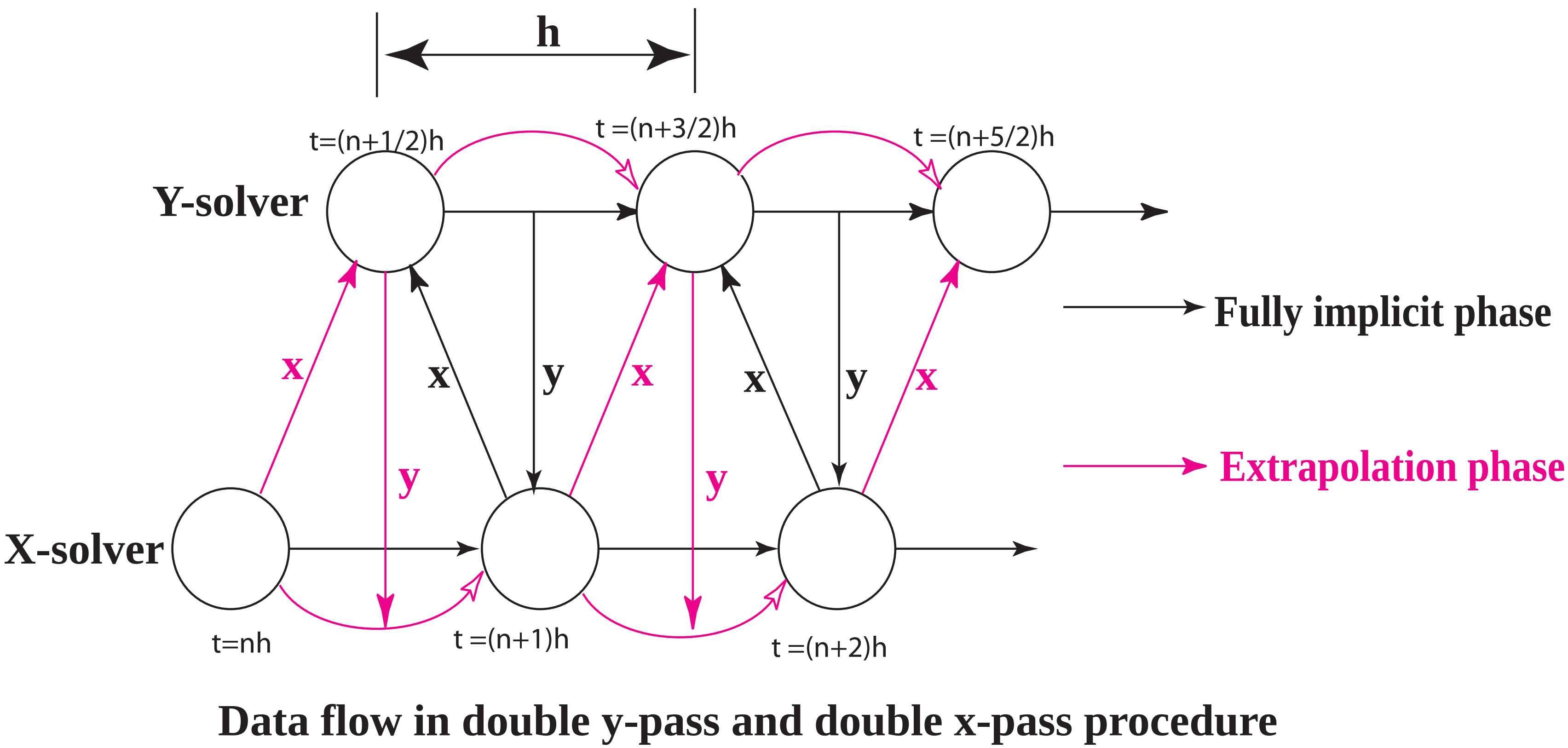

Fig. 2 Double pass staggered algorithm for a tightly coupled problem

The double-pass algorithm sketched in Fig. 2 can summarized as follows:

1. Assume that a double-pass solution of x_2^n and a single-pass solution of $y_1^{n+1/2}$ available.
2. Using $y_1^{n+1/2}$, obtain a single-pass solution of x_1^{n+1}.
3. Using $\bar{x}^{n+1/2} = \frac{1}{2}(x_1^{n+1} + x_2^n)$, obtain the double-pass solution of $y_2^{n+1/2}$.
4. Using x_1^{n+1}, obtain a single-pass solution of $y_1^{n+3/2}$.
5. Using $\bar{y}^{n+1} = \frac{1}{2}(y_2^{n+1/2} + y_1^{n+3/2})$, obtain a double-pass solution of x_2^{n+1}.
6. With the initialization of $\{y_1^{n+3/2}, x_2^{n+1}\} \rightarrow \{y_1^{n+1/2}, x_2^n\}$, or $\{t = nh \rightarrow t = (n+1)h\}$, go to step 1 and repeat the integration step.

Stability analysis of the above double-pass staggered procedure is somewhat involved and will not be treated here. The conclusion of such multi-pass correctional simulation procedures usually leads to an improvement in stability margin and occasionally attains unconditional stability. It should be noted that the stability limits of an n-pass staggered procedure would not yield any advantage, except perhaps accuracy improvements, unless the n-pass algorithm extends the stability limits by

$$h \leq mc/\mu, \quad m > n \tag{13}$$

where c is the stability limit for a single-pass staggered procedure.

In what follows we present a stabilization by physics-based augmentation.

Stabilization via physics-based augmentation

Stabilization via stiffly A-stable formulas and n-pass correctional steps discussed in the preceding sections do offer improvements in stability limits to a varying degrees. Nevertheless, they do not guarantee unconditional stability which is almost a mandatory requirement for tightly coupled stiff multi-physics simulations.

While *damping* may not offer stabilization for explicit methods, it does extend the stability limits of implicit methods qualitatively in a similar way as the stiffly A-stable formulas. However, artificial damping degrades accuracy of the solution. Recalling the root loci plots of the analytical model problem, we observe that the system possesses an intrinsic damping as the *coupling strength* increases. Hence, we explore to utilize the physically inherent system damping to *stabilize* the staggered solution procedure.

To this end, let us recall the modal equation of the tightly coupled structure acoustic equation:

$$\begin{aligned} \dot{y} + \mu y &= \rho c \ddot{x}, \quad \mu = \rho c a / m_f \\ \ddot{x} + \omega^2 x &= -\frac{m\mu}{\rho c} y, \quad \omega^2 = k_s / m_s, \quad m = m_f / m_s \end{aligned} \tag{14}$$

First, let us substitute $\ddot{x}$ from the second equation into the first to obtain the following augmented equation:

$$\begin{aligned} \dot{y} + (1+m)\mu y &= -\rho c \omega^2 x \\ \ddot{x} + \omega^2 x &= -\frac{m\mu}{\rho c} y \end{aligned} \tag{15}$$

Notice that equations (14) and (15) are physically the identical equation. However, the left hand side of the pressure equation (y-equation) in equation (15) is modified as with the right hand coupling term. In particular, its homogeneous part given by

$$\dot{y} + (m+1)\mu y = 0, \quad m > 0 \tag{16}$$

has clearly increased its response time constant. It is this increase in time constant that stabilize the staggered computational procedure.

Let us apply the one-pass staggered procedure to the *augmented* coupled physics model equation (15) as follow:

$$
\begin{aligned}
&3y^{n+1} - 4y^{n} + y^{n-1} + 2h(1+m)\mu y^{n+1} + 2h\rho c\, \omega^2 x^{n+1} = 0 \\
&x^{n+1} - x^{n} - \frac{h}{2}(\dot{x}^{n+1} + \dot{x}^{n}) = 0 \\
&\dot{x}^{n+1} - \dot{x}^{n} - \frac{h}{2}(\ddot{x}^{n+1} + \ddot{x}^{n}) = 0 \\
&\ddot{x}^{n+1} + \omega^2 x^{n+1} + \frac{m\mu}{\rho c} y_p^{n+1} = 0 \\
&y_p^{n+1} = (1+\alpha) y^{n} - \alpha y^{n-1}
\end{aligned}
\tag{17}
$$

To assess the computational stability of the above difference equation set, we seek the solution of the form:

$$\begin{Bmatrix} y^{n+1} \\ x^{n+1} \\ \dot{x}^{n+1} \\ \ddot{x}^{n+1} \end{Bmatrix} = \lambda \begin{Bmatrix} y^{n} \\ x^{n} \\ \dot{x}^{n} \\ \ddot{x}^{n} \end{Bmatrix} \tag{18}$$

Substituting this into the difference equation (17) yields

$$\begin{bmatrix} \hat{\rho}(\lambda) + (1+m)h\mu\hat{\sigma}(\lambda) & \rho c h\omega^2\hat{\sigma}(\lambda) & 0 & 0 \\ 0 & \rho(\lambda) & h\sigma(\lambda) & 0 \\ 0 & 0 & \rho(\lambda) & h\sigma(\lambda) \\ \frac{m\mu}{\rho c}e(\lambda) & \lambda\omega^2 & 0 & \lambda \end{bmatrix} \begin{Bmatrix} y^{n} \\ x^{n} \\ \dot{x}^{n} \\ \ddot{x}^{n} \end{Bmatrix} = \mathbf{0} \tag{19}$$

where

$$\begin{aligned} &\hat{\rho}(\lambda) = (3\lambda^2 - 4\lambda + 1)/\lambda, \quad \hat{\sigma}(\lambda) = 2\lambda \\ &\rho(\lambda) = \lambda - 1, \quad \sigma(\lambda) = \tfrac{1}{2}(\lambda + 1), \quad e(\lambda) = (1+\alpha) - \frac{\alpha}{\lambda} \end{aligned} \tag{20}$$

The characteristic equation of the above difference equation set is found as

$$\begin{aligned}\lambda[\hat{\rho}(\lambda)+(1+m)h\mu\hat{\sigma}(\lambda)][\rho^2(\lambda)+h^2\omega^2\sigma^2(\lambda)]\\ -m(\mu h)(\omega h)^2\sigma^2(\lambda)\hat{\sigma}(\lambda)e(\lambda)=0\end{aligned} \tag{21}$$

We carry out a quantitative stability analysis via the Routh-Hurwitz criterion by transforming λ via

$$\lambda=\frac{1+z}{1-z} \tag{22}$$

to obtain the following z-polynomial equation:

$$\begin{aligned}[4(1+2z)z+4(1+m)h\mu(1+z)^2][(2z)^2+h^2\omega^2]\\ -2m(\mu h)(\omega h)^2(1-z)[1+(1+2\alpha)z]=0\end{aligned} \tag{23}$$

which can be rearranged as

$$\begin{aligned}
&16[2+(1+m)\mu h]z^4 + 16[1+2(1+m)\mu h]z^3 \\
&+[(\omega h)^2\,(8+(4+(6+2\alpha)m)(\mu h)) + 16(\mu h)(1+m)]z^2 \\
&+2(\omega h)^2[4+(8+8m-4\alpha m)(\mu h)]z + (4+2m)(\omega h)^2(\mu h) = 0
\end{aligned} \tag{24}$$

whose roots lie in the left hand z-plane provided

$$\alpha \leq 2 \tag{25}$$

Luckily, the physics-based damping augmentation has stabilized the staggered procedure. For implementation detail, a recent paper by J. A. DeRuntz should be consulted as posted on the lecture website.