Preliminary Study of 1D Thermal-Hydraulic System Analysis Code Using the Higher-Order Numerical Scheme

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# CONTENTS





# Background

#### Reactor system analysis codes

- MARS-KS, RELAP5, COBRA-TF, TRACE and SPACE codes..
- has been developed for the realistic & best-estimate thermal-hydraulic analysis of nuclear reactor system.
- Assessment tool for the safety and conservativeness of the nuclear system
- Semi-implicit method for the time integration scheme
- First order numerical methods in both space and time discretization
  - Donor cell scheme (1<sup>st</sup> order Upwind scheme)
- Widely applied in CFD calculations due to simplicity, high stability
- However, 1<sup>st</sup> order numerical scheme can lead to excessive numerical diffusion!

### Numerical diffusion problem

- Severe problem in the 1<sup>st</sup> order numerical scheme
- Make the gradients to be smooth in the regions where the gradients should be steep
- Therefore, the accuracy of code can be deteriorated.

### Higher order schemes

- FLUENT, Star-CCM+, CFX etc.
- QUICK scheme, Lax-Wendroff scheme, High resolution scheme etc.
- The Taylor series truncation error is decreased because of higher order of error terms
- Numerical diffusion errors can be minimized



# Background

#### Next generation nuclear system safety analysis code •••

#### RFI AP7

- ✓ INL(Idaho National Lab.)
- 2<sup>nd</sup> order accurate temporal and spatial discretization
- fully implicit method & fully coupled method
  - PCICE-FFM scheme •
  - JFNK method •
  - Point implicit method
- TRACE
  - $\checkmark$ Oak Ridge National Lab.
  - Centeral difference scheme, 2<sup>nd</sup> order upwind scheme
  - Non-linear flux limiters MUSCL, Van Leer, Van Albada etc.
- COBRA-TF
  - Univ. Massachusetts Lowell & Oak Ridge National Lab.
  - 2<sup>nd</sup> order Lax-Wendroff scheme
  - Non-linear flux limiter Van Albada  $\checkmark$

#### **RFI AP-7** Timeline





Lax-Wendroff

#### Results comparison of 1<sup>st</sup> order scheme and 2<sup>nd</sup> order scheme in **COBRA-TF**

Source : Hongbin Zhang et al., RELAP7 Code Development Status Update and Future Plan, 2013

Code Development Status Update and KAIS





# **Objective & Plan**

#### Research Objective

- To see the applicapability of higher-order numerical scheme in the nuclear system safety analysis code.
- To evaluate numerical accuracy of higher-order numerical schemes.
- To identify the change of stability of higher-order numerical schemes.

#### Research Plan

- Separate single phase transient analysis code which is possible to calculate in 1st order and 2nd order scheme is built in MATLAB
  - ✓ It is impossible to implement directly 2nd order scheme in MARS-KS which is reference code for this study.
  - In this study, all of test cases is limited in single phase to see only the effect of 1st order and 2nd order scheme.
- By modeling the simple pipe flow, numerical accuracy and stability of higher-order numerical schemes are evaluated.
  - ✓ By using 2nd norm, the numerical accuracy is compared as increasing the mesh size and higher-order schemes.
  - ✓ The maximum Courant number is compared to identify the change of stability.





# **Numerical Test**

- Single phase pipe flow with sine pulse of temperature
  - Description



- ✓ Sensitivity test depending on the higher-order schemes and mesh number
  - 1<sup>st</sup> order in temporal and spatial (1T1S)
  - 1<sup>st</sup> order in temporal and 2<sup>nd</sup> order in spatial (1T2S)
  - 2<sup>nd</sup> order in temporal and 1<sup>st</sup> order in spatial (2T1S)
  - 2<sup>nd</sup> order in temporal and 2<sup>nd</sup> order in temporal (2T2S)

mesh number : 20 / 40 / 80





- Single phase pipe flow with sine pulse of temperature
  - Pulse width = 5sec & Interval = 1.5sec

#### (a) MARS vs 1T1S





- Single phase pipe flow with sine pulse of temperature
  - Pulse width = 5sec & Interval = 1.5sec

(b) Higher order sensitivity in mesh 20







- Single phase pipe flow with sine pulse of temperature
  - Pulse width = 5sec & Interval = 1.5sec

(c) Higher order sensitivity in mesh 40

(d) Higher order sensitivity in mesh 80





- Single phase pipe flow with sine pulse of temperature
  - Pulse width = 6sec & Interval = 0sec

#### (a) MARS vs 1T1S





#### Single phase pipe flow with sine pulse of temperature

Pulse width = 6sec & Interval = 0sec

#### (b) Higher order sensitivity in mesh 20







#### Single phase pipe flow with sine pulse of temperature

Pulse width = 6sec & Interval = 0sec

(c) Higher order sensitivity in mesh 40

#### (d) Higher order sensitivity in mesh 80







# Table.1 Maximum Courant number of NTS codesin case of pulse width 5sec and interval 1.5sec

|         | 1T1S   | 1T2S   | 2T1S   | 2T2S   |
|---------|--------|--------|--------|--------|
| Mesh 20 | 1.0    | 0.27   | 0.75   | 0.14   |
| Mesh 40 | 1.0224 | 0.27   | 0.6498 | 0.136  |
| Mesh 80 | 1.0147 | 0.248  | 0.632  | 0.124  |
| Average | 1.0124 | 0.2627 | 0.6773 | 0.1333 |

Table.2 Maximum Courant number of NTS codes in case of pulse width 6sec and interval 0sec

|         | 1T1S   | 1T2S   | 2T1S   | 2T2S   |
|---------|--------|--------|--------|--------|
| Mesh 20 | 0.9988 | 0.2628 | 0.7687 | 0.1349 |
| Mesh 40 | 0.9997 | 0.2499 | 0.6398 | 0.124  |
| Mesh 80 | 0.9999 | 0.26   | 0.6119 | 0.128  |
| Average | 0.9995 | 0.2576 | 0.6735 | 0.129  |

### Summary

### Summary

- The 2<sup>nd</sup> order upwind scheme and 2<sup>nd</sup> order backward Euler scheme are implemented for the spatial and temporal scheme.
- In the 1<sup>st</sup> order scheme, the temperature distribution is severely distorted due to the numerical diffusion.
- When the only 2<sup>nd</sup> order sheme in time are applied, the results are not much different from the 1<sup>st</sup> order scheme in both time and space.
- In the 2<sup>nd</sup> order spatial scheme, it is identified that the accuracy is improved and the numerical dispersion can be occured.
- When the 2nd order scheme in time and space are applied together, the numerical dispersion is more severe and the lowest Courant number is indicated.

### Conclusions

- In terms of the accuracy of the code, the 2<sup>nd</sup> order spatial scheme is more influenced than the 2<sup>nd</sup> order temporal scheme.
- The 2<sup>nd</sup> order spatial scheme is more rigid than the 2<sup>nd</sup> order temporal scheme due to low maximum Courant number.
- In the 2<sup>nd</sup> order spatial scheme, the numerical dispersion can be occurred.





### **Further works**

#### Further works

- For improving the applicability of the higher order scheme in thermal hydraulic system analysis code, various higher order numerical schemes are needed to evaluate numerical accuracy and efficiency.
  - ✓ 2<sup>nd</sup> order Lax-Wendroff method, QUICK scheme etc..
- For increasing the stability of the higher order scheme, the flux limiters will be applied and evaluate performance and applicability.
  - ✓ MUSCL, Van Leer, OSPRE, Van Albada etc..
- Finally, the optimum higher order numerical scheme will be evaluated and the application methodology will be developed.



# THANK YOU FOR YOUR ATTENTION!



# Appendix

#### Spatial Discretization schemes

Upwind scheme (Donor cell scheme) – 1<sup>st</sup> order

- ✓ In steady state,

$$F_e \phi_e - F_w \phi_w = D_e (\phi_E - \phi_P) - D_w (\phi_P - \phi_W)$$
$$F = \rho u A \qquad D = \frac{\Gamma A}{\delta x}$$

Rearranging equation,

 $a_P\phi_P=a_W\phi_W+a_E\phi_E$ 

For positive flow direction

 $a_w = D_w + F_w$   $a_E = D_e$ 

 $a_P = a_W + a_E + (F_e - F_w)$ 

- Widely applied in early CFD calculations due to simplicity, high stability
- ✓ Numerical diffusion problem
- Other 1<sup>st</sup> order scheme Power law scheme, Hybrid scheme etc.



✓ For negative flow direction  $a_P = a_W + a_E + (F_e - F_w)$ 

$$a_w = D_w \qquad a_E = D_e - F_e$$

convergence, 1993



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# Appendix

- Spatial Discretization schemes
  - Upwind scheme (Donor cell scheme) 2<sup>nd</sup> order

The value at a cell face is determined depending on the flow direction



✓ Implemented in ANSYS FLUENT 12.0, CFX, Star CCM+ etc.

Source : H.K. Versteeg, et al., *An introduction to computational fluid dynamics*, 1995

✓ Numerical dispersion problem

Other higher order scheme – QUICK shceme, Lax-Wendroff scheme, 3<sup>rd</sup> order MUSCL scheme etc.



Source : Ling Zou et al., *Applications of high-resolution spatial discretization scheme and Jacobian-free Newton-Krylov method in two=phase flow problems*, 2015





# Appendix

Time Discretization schemes

#### Backward Euler scheme – 1<sup>st</sup> order

✓ Stable implicit time integration method

$$\frac{\partial u(x,t)}{\partial t} + a \frac{\partial u(x,t)}{\partial x} = 0$$
$$\left(\frac{\partial u(x,t)}{\partial t}\right)_{n+1} = \frac{u_i^{n+1} - u_i^n}{\Delta t} + \frac{\Delta t}{2} \left(\frac{\partial^2 u}{\partial t^2}\right)_{n+1} + O(\Delta t^2)$$

#### Backward Euler scheme – semi-implicit

✓ To produce an approximate discrete solution by iterating  

$$v_{n+1} = v_n + g(t_n, x_n)\Delta t$$
  
 $x_{n+1} = x_n + f(t_n, v_{n+1})\Delta t$ 

 Convective terms in the mass and energy equations, pressure gradient term in the momentum equation, and the compressible work term in the energy equation evaluated at the new time level

#### Backward Euler scheme – 2<sup>nd</sup> order

✓ Implemented in RELAP7

$$\left(\frac{\partial u(x,t)}{\partial t}\right)_{n+1} = \frac{3u_i^{n+1} - 4u_i^n + u_i^{n-1}}{2\Delta t} + O(\Delta t^2)$$





# **Appendix – NTS code**

#### > NPNP Transient System code

- ✓ Identical solver to MARS code (Semi-implicit)
- Single phase governing equations
- Option 1<sup>st</sup> order in temporal and spatial
   1<sup>st</sup> order in temporal and 2<sup>nd</sup> order in spatial
   2<sup>nd</sup> order in temporal and 1<sup>st</sup> order in spatial
   2<sup>nd</sup> order in temporal and 2<sup>nd</sup> order in temporal
- Dittus-Boelter correlation for heat transfer coefficient in single phase

$$HTC = 0.023 \frac{k_{\nu}}{D_{H}} (\frac{G_{\nu} D_{H}}{\mu_{\nu}})^{0.8} (\text{Pr}_{\nu})^{0.4}$$

 Friction factor model (Colebrook-White correlation for turbulent friction factor)

$$\begin{split} \lambda_{\rm L} &= \frac{64}{{\rm Re}\Phi_{\rm g}}, \quad 0 \leq {\rm Re} \leq 2200 \\ \lambda_{\rm L,\,T} &= \left(3.75 - \frac{8250}{{\rm Re}}\right) (\lambda_{\rm T,\,8000} - \lambda_{\rm L,\,2200}) + \lambda_{\rm L,\,2200} \quad \mbox{ for } 2200 < {\rm Re} < 3000 \\ \frac{1}{\sqrt{\lambda_{\rm T}}} &= -2\log_{10} \bigg\{ \frac{\epsilon}{3.7{\rm D}} + \frac{2.51}{{\rm Re}} \Big[ 1.14 - 2\log_{10} \Big( \frac{\epsilon}{{\rm D}} - \frac{21.25}{{\rm Re}^{0.9}} \Big) \Big] \bigg\} \end{split}$$









# **Appendix – NTS governing equations**

#### > NPNP Transient System code – Hydrodynamic solver

- 1<sup>st</sup>-order accuracy difference & Semi-implicit scheme in single phase governing equation
  - Convective term in the mass and energy equation
  - Pressure gradient term in the momentum equation
  - Compressible work term in the energy equation
- Governing equations Two phase, Two field model
  - ✓ Mass Continuity

$$\frac{\partial}{\partial t}(\alpha_{f}\rho_{f}) + \frac{1}{A}\frac{\partial}{\partial x}(\alpha_{f}\rho_{f}v_{f}A) = \mathbf{V}_{f}$$

$$\frac{\partial}{\partial t}(\alpha_{g}\rho_{g}) + \frac{1}{\underline{A}\partial x}(\alpha_{g}\rho_{g}\nabla_{g}A) = \underline{\Gamma}_{g}$$

$$\alpha_{f}\rho_{f}A\frac{\partial v_{f}}{\partial t} + \frac{1}{2}\alpha_{f}\rho_{f}A\frac{\partial v_{f}^{2}}{\partial x} = -\alpha_{f}A\frac{\partial P}{\partial x} + \alpha_{f}\rho_{f}B_{x}A - (\alpha_{f}\rho_{f}A)FWF(v_{f})$$

$$\alpha_{g}\rho_{g}A\frac{\partial v_{g}}{\partial t} + \frac{1}{2}\alpha_{g}\rho_{g}A\frac{\partial v_{g}^{2}}{\partial x} = -\alpha_{g}A\frac{\partial P}{\partial x} + \alpha_{g}\rho_{g}B_{x}A - (\alpha_{g}\rho_{g}A)FWG(v_{g})$$

$$(-)\Gamma_{g}A(v_{fI} - v_{f}) - (\alpha_{f}\rho_{f}A)FIF(v_{f} - v_{g})$$

$$+ \Gamma_{g}A(v_{gI} - v_{g}) - (\alpha_{g}\rho_{g}A)FIG(v_{g} - v_{f})$$

$$+ \Gamma_{g}A(v_{gI} - v_{g}) - (\alpha_{g}\rho_{g}A)FIG(v_{g} - v_{f})$$

$$-C\alpha_{f}\alpha_{g}\rho_{m}A\left[\frac{\partial(v_{f} - v_{g})}{\partial t} + v_{g}\frac{\partial v_{f}}{\partial x} - v_{f}\frac{\partial v_{g}}{\partial x}\right]$$

$$-C\alpha_{g}\alpha_{f}\rho_{m}A\left[\frac{\partial(v_{g} - v_{f})}{\partial t} + v_{f}\frac{\partial v_{g}}{\partial x} - v_{g}\frac{\partial v_{f}}{\partial x}\right]$$

✓ Energy Conservation

$$\frac{\partial}{\partial t}(\alpha_{f}\rho_{f}U_{f}) + \frac{1}{\underline{A}\partial x}(\alpha_{f}\rho_{f}U_{f}v_{f}A) = -P\frac{\partial\alpha_{f}}{\partial t} - \frac{P}{\underline{A}\partial x}(\alpha_{f}v_{f}A) + Q_{wf} + Q_{if} = P_{ig}h_{f}^{*} - \Gamma_{w}h_{f}^{'} + DISS_{f}$$

$$\frac{\partial}{\partial t}(\alpha_{g}\rho_{g}U_{g}) + \frac{1}{A}\frac{\partial}{\partial x}(\alpha_{g}\rho_{g}U_{g}V_{g}A) = -P\frac{\partial\alpha_{g}}{\partial t} - \frac{P}{A}\frac{\partial}{\partial x}(\alpha_{g}V_{g}A) + Q_{wg} + Q_{ig} + \Gamma_{ig}h_{g}^{*} + \Gamma_{w}h_{g} + DISS_{g}$$





# **Appendix – NTS Hydrodynamic solver**

#### > NPNP Transient System code – Hydrodynamic solver

Momentum Conservation

 $\checkmark$ 

State relations

$$\alpha_{i}\rho_{i}A\frac{\partial v_{i}}{\partial t} + \frac{1}{2}\alpha_{i}\rho_{i}A\frac{\partial v_{i}}{\partial x}^{2} = -\alpha_{i}A\frac{\partial p}{\partial x} + \alpha_{i}\rho_{i}B_{a}A - (\alpha_{i}\rho_{i}A)FWF(v_{i})$$

$$(-)\Gamma_{a}A(v_{i}-v_{i}) + (-\alpha_{i}\rho_{i}A)FWF(v_{i})$$

$$(-)\Gamma_{a}A(v_{i}-v_{i}) + (-\alpha_{i}\rho_{i}A)FWF(v_{i}-v_{i})$$

$$(-)\Gamma_{a}A(v_{i}-v_{i}A)FWF(v_{i}-v_{i})$$

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$$(-)\Gamma_{a}A(v_{i}-v_{i}A)FWF(v_{i}A)FWF(v_{i}A)FWF(v_{i}A)FWF(v_{i}A)FWF(v_{i}A)FWF$$

$$\frac{\partial}{\partial t}(\alpha_{f}\rho_{f}U_{f}) + \frac{1}{\underline{A\partial x}}(\alpha_{f}\rho_{f}U_{f}V_{f}A) = -P\frac{\partial\alpha_{f}}{\partial t} - \frac{P}{\underline{A\partial x}}(\alpha_{f}v_{f}A) + Q_{wf} + D_{i}S_{f}$$

$$X\left(\frac{\partial\rho}{\partial P}\right)\delta P_{i+\frac{1}{2}} + Y\left(\frac{\partial\rho}{\partial T}\right)\delta T_{i+\frac{1}{2}} = D + E\left(\delta P_{i+\frac{3}{2}} - \delta P_{i+\frac{1}{2}}\right) + F\left(\delta P_{i+\frac{1}{2}} - \delta P_{i-\frac{1}{2}}\right)$$



# Appendix – NTS Hydrodynamic solv

#### > NPNP Transient System code – Hydrodynamic solver

Pressure difference matrix

$$\bar{A} \begin{pmatrix} \delta P \\ \delta T \end{pmatrix} = \bar{D} + \bar{E} \left( \delta P_{i+\frac{3}{2}} - \delta P_{i+\frac{1}{2}} \right) - \bar{F} \left( \delta P_{i+\frac{1}{2}} - \delta P_{i-\frac{1}{2}} \right)$$

 Multiplying above matrix by  $A^{-1}$  results in a single equation involving pressures.

$$\begin{split} &-\bar{A}^{-1}\bar{F}\delta P_{i-\frac{1}{2}} + (1+\bar{A}^{-1}\bar{E}+\bar{A}^{-1}\bar{F})\delta P_{i+\frac{1}{2}} - \bar{A}^{-1}\bar{E}\delta P_{i+\frac{3}{2}} = \bar{A}^{-1}\bar{D}\\ &\delta T_{i+\frac{1}{2}} = \bar{A}^{-1}\bar{D} + \bar{A}^{-1}\bar{E}\left(\delta P_{i+\frac{3}{2}} - \delta P_{i+\frac{1}{2}}\right) - \bar{A}^{-1}\bar{F}\left(\delta P_{i+\frac{1}{2}} - \delta P_{i-\frac{1}{2}}\right) \end{split}$$

- ✓ N X N sparse matrix in a system containing N volumes
- Pressure difference of each volume is substituted into eq.(2) and the velocity equations.



### **Appendix – NTS Heat structure solver**

#### > NPNP Transient System code – Heat structure solver

Heat Conduction

$$\iiint_{\mathbb{V}} \rho(T,\overline{x}) \frac{\partial T}{\partial t}(\overline{x},t) d\mathbb{V} = \iint_{\mathbb{S}} k(T,\overline{x}) \overline{\mathbb{V}} T(\overline{x},t) \bullet d\overline{s} + \iiint_{\mathbb{V}} S(\overline{x},t) d\mathbb{V}$$

$$\rho \frac{T_i^{n+1} - T_i^n}{\Delta t} = k \frac{r_{i+\frac{1}{2}} \left(\frac{T_{i+1} - T_i}{\Delta r}\right) - r_{i-\frac{1}{2}} \left(\frac{T_i - T_{i-1}}{\Delta r}\right)}{r_i \Delta r} + S$$
$$= \xi_i$$

✓ Crank-Nicholson method (w = 
$$\frac{1}{2}$$
)

