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)

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





![](_page_19_Picture_11.jpeg)

![](_page_19_Picture_12.jpeg)

# **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

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

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

![](_page_20_Picture_15.jpeg)

![](_page_20_Picture_16.jpeg)

# **Appendix – NTS Hydrodynamic solver**

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

Momentum Conservation

 $\checkmark$ 

State relations

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

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

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

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

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

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

![](_page_21_Picture_5.jpeg)

# 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.

![](_page_22_Figure_9.jpeg)

### **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 = 
$$\frac{1}{2}$$
)

![](_page_23_Figure_7.jpeg)