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MULTIPLE BALANCE TIME-DISCRETIZATION

A ROBUST SECOND-ORDER METHOD FOR MULTI-PHYSICS SIMULATIONS

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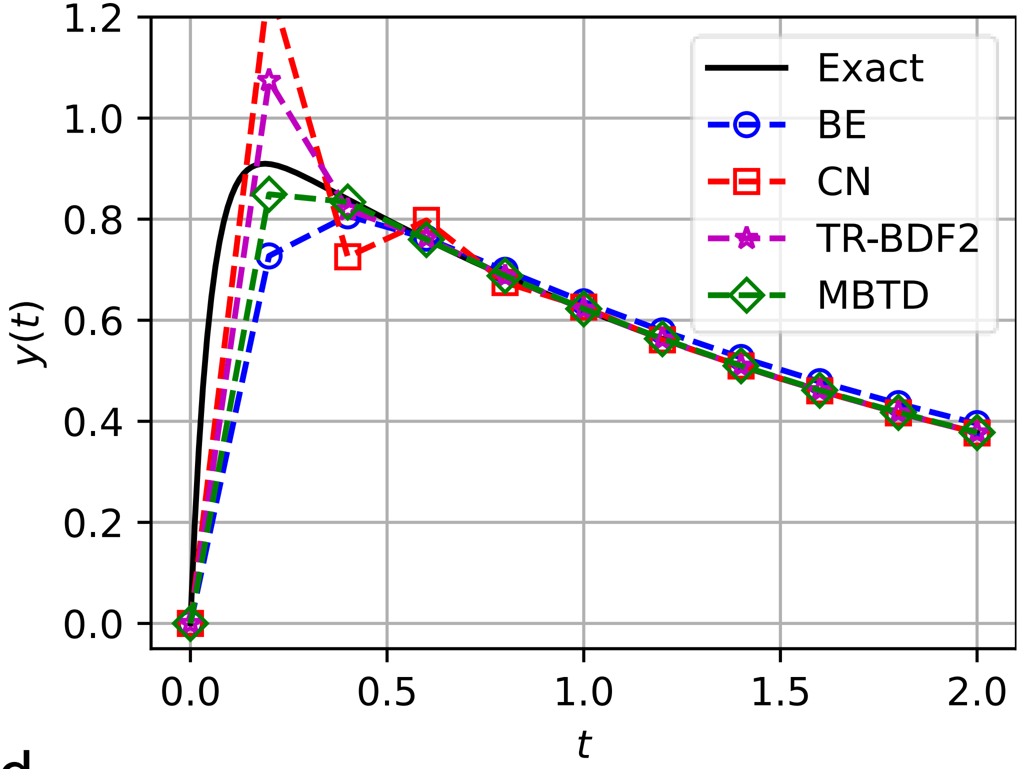
Dilemma of choosing accuracy (CN) or robustness (BE)

- The widely used **time-stepping** θ-Method:
  - Backward Euler (**BE**, $\theta = 1$)
    - ➢Robust, but 1st-order accurate
  - Crank-Nicholson (**CN**, $\theta = 0.5$)
    - ➢2nd-order accurate, but NOT robust
- **Robust:** stable & free of spurious oscillations
- **Spurious oscillations** yield unphysical solutions and may jeopardize feedback
- Adaptive-stepping benefits from robust method
- **Multiple Balance Time-Discretization (MBTD)** is **robust** and **2nd-order accurate**



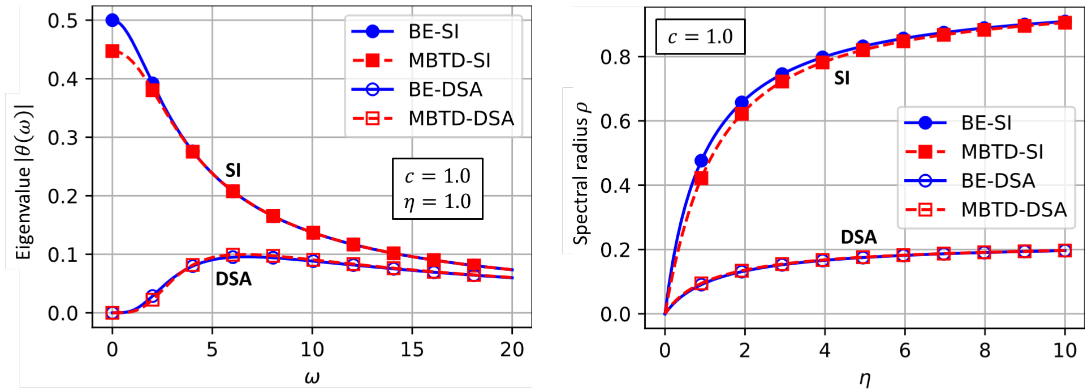
Numerical solutions of a test problem

MBTD is higher-order alternative to the robust BE

Studies on MBTD

Application on **single-physics neutron transport**:

- Preliminary study [Variansyah 2020]
- More detailed investigation [Variansyah 2021]
  - Strategies for solving *coupled balance equations*
  - Develop and Fourier-analyze MBTD-SI & MBTD-DSA
  - SN & MOC
  - Delayed neutron approximations



Fourier analysis

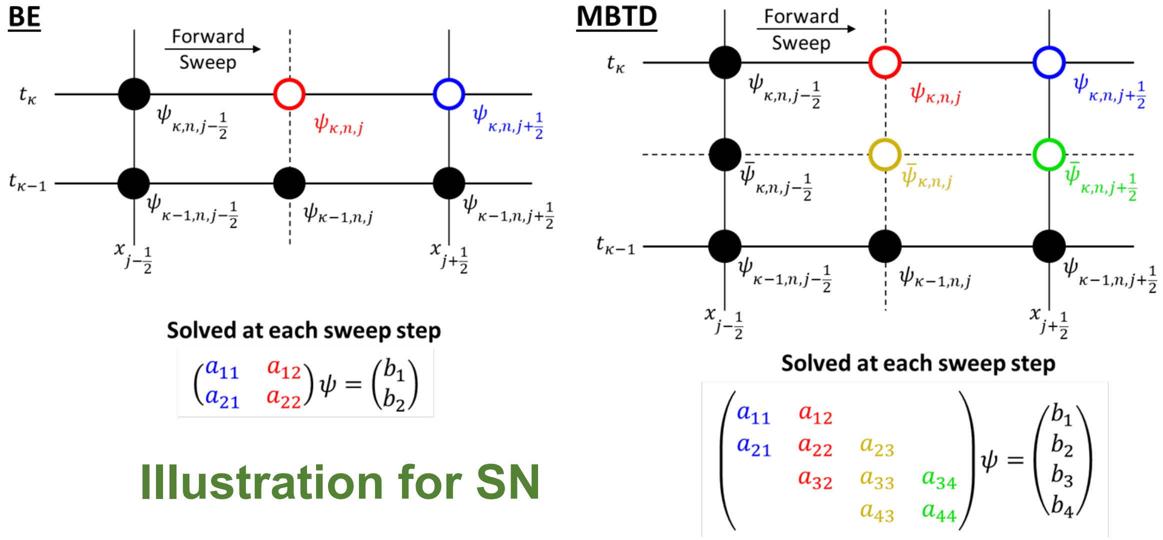


Illustration for SN

This paper: preliminary study for multi-physics application

Outline

1. MBTD
   Linear & non-linear problems
   Connection to Mid-point and Runge-Kutta
2. Multi-physics *tight-coupling* for MBTD
3. Test problem and numerical results

MBTD – Coupled Balance Equations

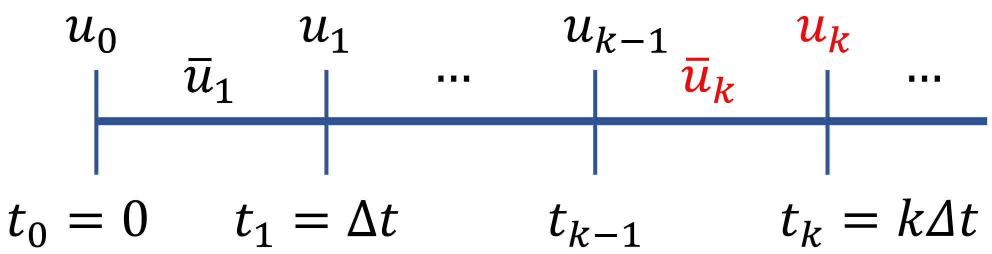
Time-stepping

$$\frac{\partial u}{\partial t} + \boldsymbol{L}u(t) = 0$$

$$\frac{\color{red}{u_k} - u_{k-1}}{\Delta t} + \boldsymbol{L}\color{red}{\bar{u}_k} = 0$$

Time-edge solution

Time-average solution



At each time-step:
1 equation, 2 unknowns
→ Need **auxiliary equation**

θ-Method

$$\color{red}{\bar{u}_k} = \begin{cases} u_{k-1}, & \textbf{FE,} \\ \color{red}{u_k}, & \textbf{BE,} \\ \dfrac{u_{k-1} + \color{red}{u_k}}{2}, & \textbf{CN} \end{cases}$$

MBTD

Original balance

$$\begin{cases} \boxed{\dfrac{\color{red}{u_k} - u_{k-1}}{\Delta t} + \boldsymbol{L}\color{red}{\bar{u}_k} = 0,} \\ \boxed{\dfrac{\color{red}{u_k} - \color{red}{\bar{u}_k}}{\Delta t/2} + \boldsymbol{L}\color{red}{u_k} = 0} \end{cases}$$

Balance-like

MB [Morel & Larsen 90]:
- Only using the unknowns
- Exact as $\Delta t \to 0$
- As "implicit" as possible

Coupled balance equations

MBTD – Accuracy and robustness

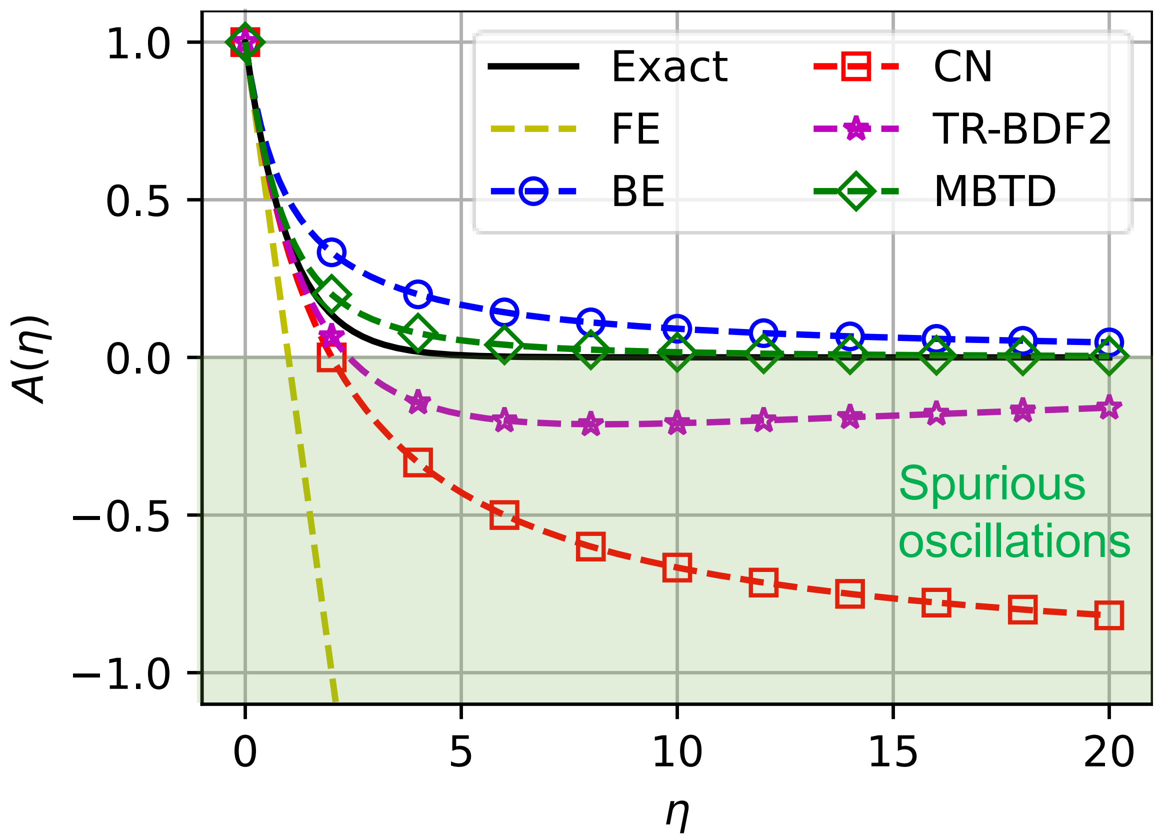
$$\frac{1}{v}\frac{d\psi}{dt} + \Sigma_t\psi(t) = 0, \qquad \psi(t) = \psi_0 e^{-v\Sigma_t t}$$

$$\psi_k = A(\eta)\psi_{k-1}, \qquad A_{\text{Exact}}(\eta) = e^{-\eta}$$

η: "**mean-free-path traveled per Δt**" $= v\Sigma_t\Delta t$

Method	Amplification factor: $A(\eta)$	Time-step error factor: $A_{\text{Exact}}(\eta) - A(\eta)$	Robustness: $0 \le A(\eta) \le 1$
FE	$1-\eta$	$\frac{1}{2}\eta^2 + O(\eta^3)$	$\eta \le 1$
BE	$\frac{1}{1+\eta}$	$-\frac{1}{2}\eta^2 + O(\eta^3)$	$\eta \ge 0$
CN	$\frac{1-\frac{1}{2}\eta}{1+\frac{1}{2}\eta}$	$\frac{1}{12}\eta^3 + O(\eta^4)$	$\eta \le 2$
MBTD	$\frac{1}{1+\eta+\frac{1}{2}\eta^2}$	$-\frac{1}{6}\eta^3 + O(\eta^4)$	$\eta \ge 0$

Amplification factor $A(\eta)$



MBTD is 2nd order accurate and robust

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Strategies for solving MBTD Coupled Balance Equations

It's straightforward to solve BE (slightly modifying SS solver)

$$\frac{u_k - u_{k-1}}{\Delta t} + \boldsymbol{L} u_k = 0$$

How do we ***efficiently*** solve MBTD coupled equations?

$$\begin{cases} \dfrac{u_k - u_{k-1}}{\Delta t} + \boldsymbol{L}\bar{u}_k = 0, \\ \dfrac{u_k - \bar{u}_k}{\Delta t/2} + \boldsymbol{L} u_k = 0 \end{cases}$$

Substitution

Correction term to BE

$$\frac{u_k - u_{k-1}}{\Delta t} + \left(\boldsymbol{L} + \frac{1}{2}\Delta t \boldsymbol{L}^2\right) u_k = 0$$

Iterative Solve

Lagging small quantity $O(\Delta t)$

$$\begin{cases} \dfrac{\bar{u}_k^{(l)} - u_{k-1}}{\Delta t} + \boldsymbol{L}\bar{u}_k^{(l)} = -\dfrac{1}{\Delta t}\left(u_k^{(l-1)} - \bar{u}_k^{(l-1)}\right) \\ \dfrac{u_k^{(l)} - \bar{u}_k^{(l)}}{\Delta t/2} + \boldsymbol{L} u_k^{(l)} = 0 \end{cases}$$

★ **Simultaneous Solve**

$$\begin{bmatrix} \boldsymbol{L} + \dfrac{1}{\Delta t}\boldsymbol{I} \end{bmatrix}$$

BE sweep

$$\begin{bmatrix} \boldsymbol{L} & \dfrac{1}{\Delta t}\boldsymbol{I} \\ -\dfrac{2}{\Delta t}\boldsymbol{I} & \boldsymbol{L} + \dfrac{2}{\Delta t}\boldsymbol{I} \end{bmatrix}$$

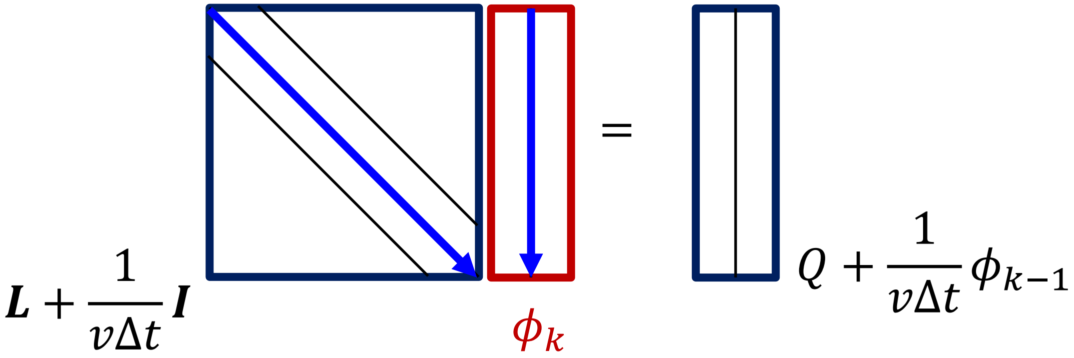
MBTD sweep

MBTD for finite-difference neutron diffusion

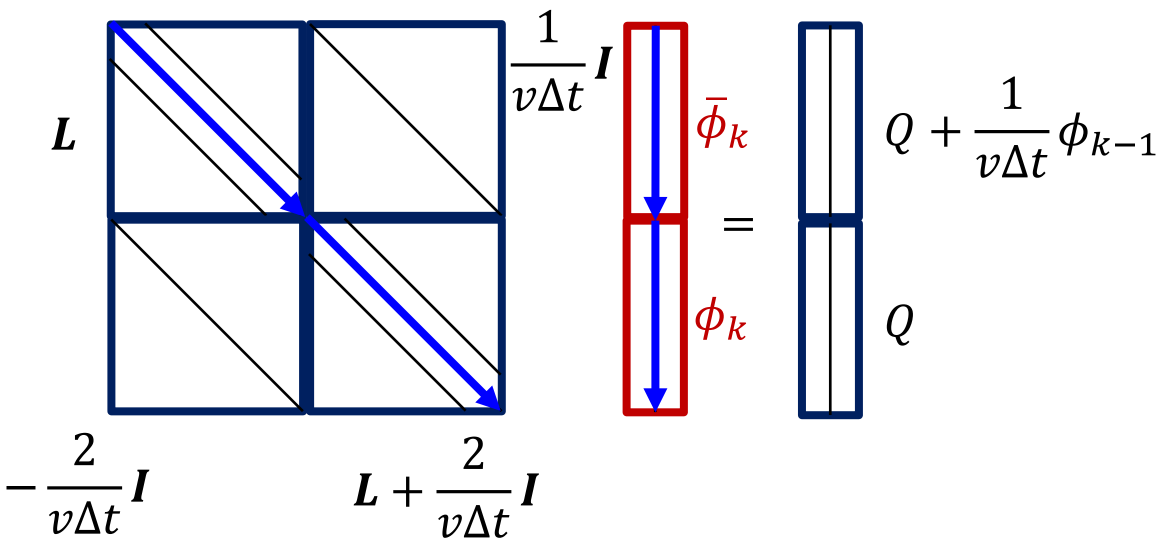
Mono-energetic homogeneous 1D-slab problem:

$$\frac{1}{v}\frac{\partial \phi}{\partial t} - D\frac{\partial^2 \phi}{\partial x^2} + \Sigma_a \phi(x,t) = \nu \Sigma_f \phi(x,t) + Q(x), \qquad 0 \le x \le X, \qquad t > 0,$$

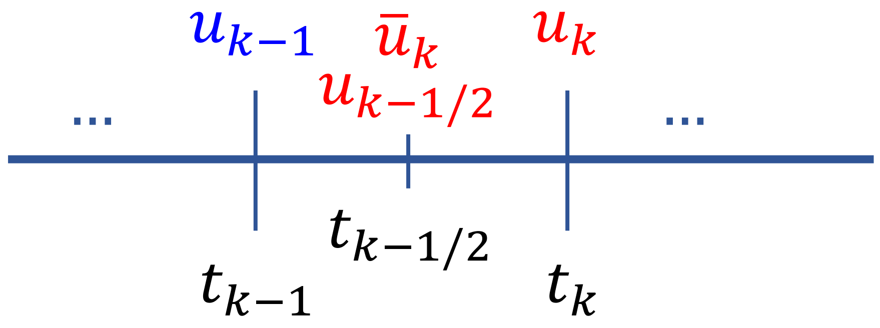
Backward Euler



MBTD



MBTD for non-linear problems



Linear problem

$$\frac{\partial u}{\partial t} + \boldsymbol{L}u(t) = 0$$

$$\begin{cases} \dfrac{u_k - u_{k-1}}{\Delta t} + \boldsymbol{L}\bar{u}_k = 0, \\ \dfrac{u_k - \bar{u}_k}{\Delta t/2} + \boldsymbol{L}u_k = 0 \end{cases}$$

Nonlinear problem

$$\frac{\partial u}{\partial t} + f[t, u(t)] = 0$$

$$\begin{cases} \dfrac{u_k - u_{k-1}}{\Delta t} + f\left(t_{k-1/2}, u_{k-1/2}\right) = 0, \\ \dfrac{u_k - u_{k-1/2}}{\Delta t/2} + f(t_k, u_k) = 0 \end{cases}$$

MBTD is a Mid-point method with “right-implicit” approximation

MBTD in Runge-Kutta form

$$\begin{cases} u_k = u_{k-1} + \Delta t \sum_{i=1}^{s} b_i f(t_{k-1} + c_i \Delta t, Y_i)\,, \\ Y_i = u_{k-1} + \Delta t \sum_{j=1}^{s} a_{ij} f\left(t_{k-1} + c_j \Delta t, Y_j\right), \qquad i = 1, 2, \dots, s \end{cases}$$

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array}$$

Butcher Tableau (method's "fingerprint")

BE	CN	Two-stage Explicit RK (Mid-point, left-explicit)	MBTD (Mid-point, right-implicit)
$\begin{array}{c\|c} 1 & 1 \\ \hline & 1 \end{array}$	$\begin{array}{c\|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array}$	$\begin{array}{c\|cc} 0 & 0 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 0 & 1 \end{array}$	$\begin{array}{c\|cc} 1/2 & 1 & -1/2 \\ 1 & 1 & 0 \\ \hline & 1 & 0 \end{array}$

We do not believe that MBTD has been used or studied before

Multi-physics tight-coupling for MBTD

Generic two-physics

$$\frac{\partial u_i}{\partial t} = f_i[t, u_1(t), u_2(t)], \qquad i = 1, 2$$

BE

$$\frac{u_{i,k} - u_{i,k-1}}{\Delta t} = f_i(t_k, u_{1,k}, u_{2,k})$$

Full-coupling	Tight-coupling	Loose-coupling (Operator Splitting)
$\frac{\vec{u}_k - \vec{u}_{k-1}}{\Delta t} = f(t_k, \vec{u}_k)$ Use non-linear solver (e.g., JFNK) $\vec{u}_k = [u_{1,k} \quad u_{2,k}]$	$\begin{cases} \frac{u_{1,k}^{(l)} - u_{1,k-1}}{\Delta t} = f_1\left(t_k, u_{1,k}^{(l)}, u_{2,k}^{(l-1)}\right), \\ \frac{u_{2,k}^{(l)} - u_{2,k-1}}{\Delta t} = f_2\left(t_k, u_{1,k}^{(l)}, u_{2,k}^{(l)}\right) \end{cases}$ Staggered (Gauss-Seidel-style) Picard Iteration	$\begin{cases} \frac{u_{1,k}^{(l)} - u_{1,k-1}}{\Delta t} = f_1\left(t_k, u_{1,k}^{(l)}, u_{2,k-1}\right), \\ \frac{u_{2,k}^{(l)} - u_{2,k-1}}{\Delta t} = f_2\left(t_k, u_{1,k}^{(l)}, u_{2,k}^{(l)}\right) \end{cases}$ Lie-Splitting Introduces $O(\Delta t)$ error…

Multi-physics tight-coupling for MBTD

BE tight-coupling

$$\begin{cases} \dfrac{u_{1,k}^{(l)} - u_{1,k-1}}{\Delta t} = f_1\left(t_k, u_{1,k}^{(l)}, u_{2,k}^{(l-1)}\right), \\ \dfrac{u_{2,k}^{(l)} - u_{2,k-1}}{\Delta t} = f_2\left(t_k, u_{1,k}^{(l)}, u_{2,k}^{(l)}\right) \end{cases}$$

MBTD tight-coupling

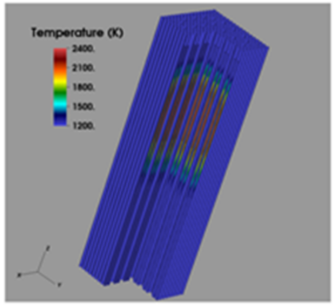
$$\begin{cases} \begin{cases} \dfrac{u_{1,k}^{(l)} - u_{1,k-1}}{\Delta t} = f_1\left(t_{k-1/2}, u_{1,k-1/2}^{(l)}, u_{2,k-1/2}^{(l-1)}\right), \\ \dfrac{u_{1,k}^{(l)} - u_{1,k-1/2}^{(l)}}{\Delta t/2} = f_1\left(t_k, u_{1,k}^{(l)}, u_{2,k}^{(l-1)}\right), \end{cases} \\ \begin{cases} \dfrac{u_{2,k}^{(l)} - u_{2,k-1}}{\Delta t} = f_2\left(t_{k-1/2}, u_{1,k-1/2}^{(l)}, u_{2,k-1/2}^{(l)}\right), \\ \dfrac{u_{2,k}^{(l)} - u_{2,k-1/2}^{(l)}}{\Delta t/2} = f_2\left(t_k, u_{1,k}^{(l)}, u_{2,k}^{(l)}\right). \end{cases} \end{cases}$$

Test problem

- Adapted from a simplified neutronics/TH SS problem [Toth, M&C 2015]

ANALYSIS OF ANDERSON ACCELERATION ON A SIMPLIFIED NEUTRONICS/THERMAL HYDRAULICS SYSTEM

A. Toth[1], C.T Kelley[1], S. Slattery[2], S. Hamilton[2], K. Clarno[2], and R. Pawlowski[3]



- 1D-slab neutron diffusion

$$\frac{1}{v}\frac{\partial \phi}{\partial t} - \frac{\partial}{\partial z}\frac{1}{3\Sigma_t(T)}\frac{\partial \phi}{\partial z} + \Sigma_a(T)\phi(z,t) = \xi\nu\Sigma_f(T)\phi(z,t)$$

- Constant-flow heat equation

$$\rho_f A_f c_{p,f}(T_f)\frac{\partial T_f}{\partial t} + 2\pi R_f h\left[T_f(z,t) - T_w(z,t)\right] = \kappa\Sigma_f(T)\phi(z,t)$$

$$\rho_w(T_w)A_w c_{p,w}(T_w)\frac{\partial T_w}{\partial t} + \dot{m}c_{p,w}(T_w)\frac{\partial T_w}{\partial z} = 2\pi R_f h\left[T_f(z,t) - T_w(z,t)\right]$$

- Temperature-dependent XS (linear interpolation)

T_f [K]	T_w [K]	$\Sigma_t(T)$ [/cm]	$\Sigma_s(T)$ [/cm]	$\nu\Sigma_f(T)$[/cm]
565	565	0.655302	0.632765	0.0283063
1565	565	0.653976	0.631252	0.0277754
565	605	0.61046	0.589171	0.0265561

$T(z,t) = \left[T_f(z,t) \quad T_w(z,t)\right]$

Initial condition: Steady state at power rate 200 MW/cm
Transient: Dropping $T_{w,in}$ from 565 to 515 K at $t = 0$

Test problem – numerical setup

- $\dot{m} = 0.3$ kg/s, $h = 0.2$ W/cm²-K, $\kappa_f = 191.4$ MeV
- $R_f = 0.5$ cm, $d = 1.3$ cm, $Z = 360$ cm
- $v = 2.2 \times 10^5$ cm/s
- Temperature-dependent ρ and c_p (UO_2, water $15.5.$ MPa) from Python-package `thermo`
- Box-scheme finite-difference (diffusion), up-wind (coolant), $J = 1800$ spatial meshes
- Multi-physics coupling relative tolerance $\varepsilon_r = 10^{-5}$
- SciPy's sparse ILU-preconditioned GMRES and MINPACK with tolerance $\varepsilon_r \times 10^{-2}$

SS initial condition

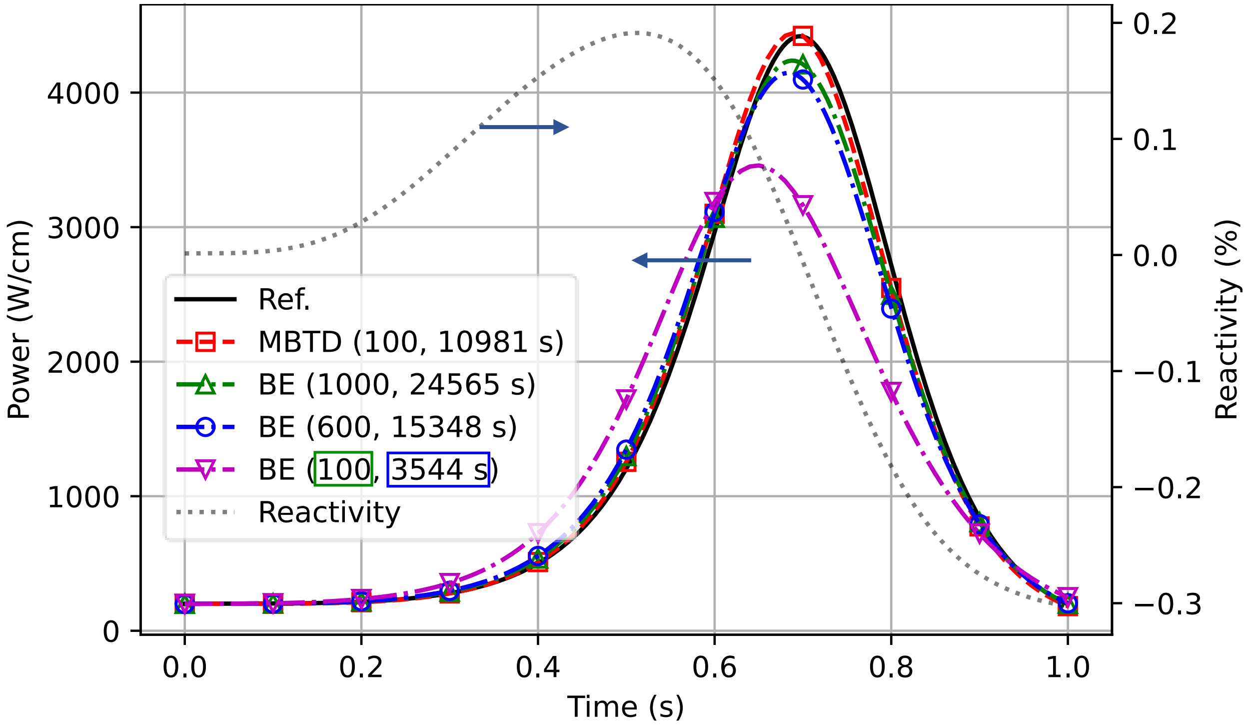
- $P = 200$ W/cm, $T_{w,in} = 565$ K
- Relaxed-Picard $(\omega = 0.5)$
- $\xi = 0.8097$, $k = 1.00001$

Transient

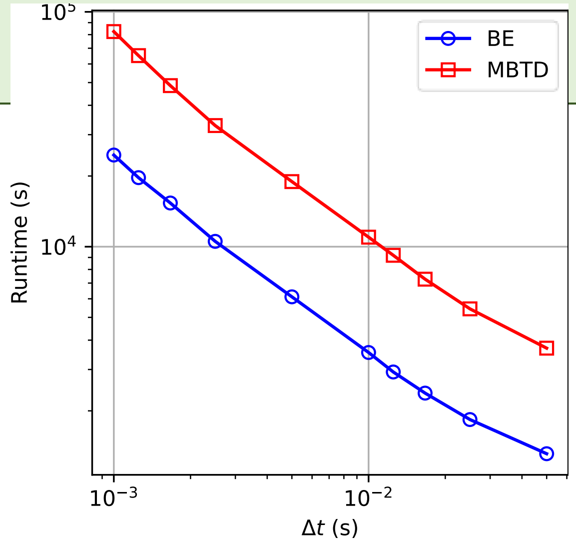
- $T_{w,in} = 565$ K $\rightarrow 515$ K at $t = 0$
- Simulated up to $t = 1$ s
- Staggered tightly-coupled BE and MBTD
  $K \in [20, 1000]$ time steps
- Reference:
  Staggered tightly-coupled CN, $K = 2000$
- Efficiency metrics:
  runtime, total power, peak power, peak time

Transient solution

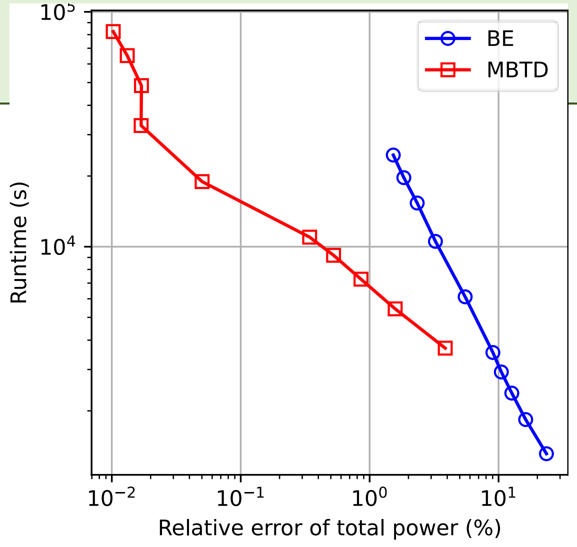
Results – MBTD and BE efficiency



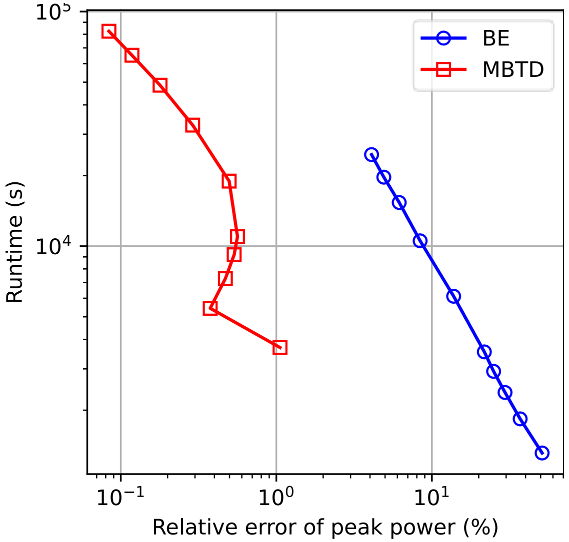
(# of time-steps, runtime)



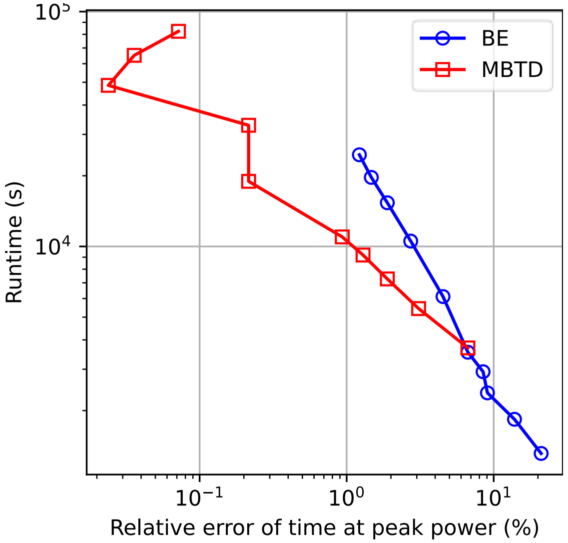
Runtime



Efficiency for Total Power



Efficiency for Peak Power



Efficiency for Peak Time

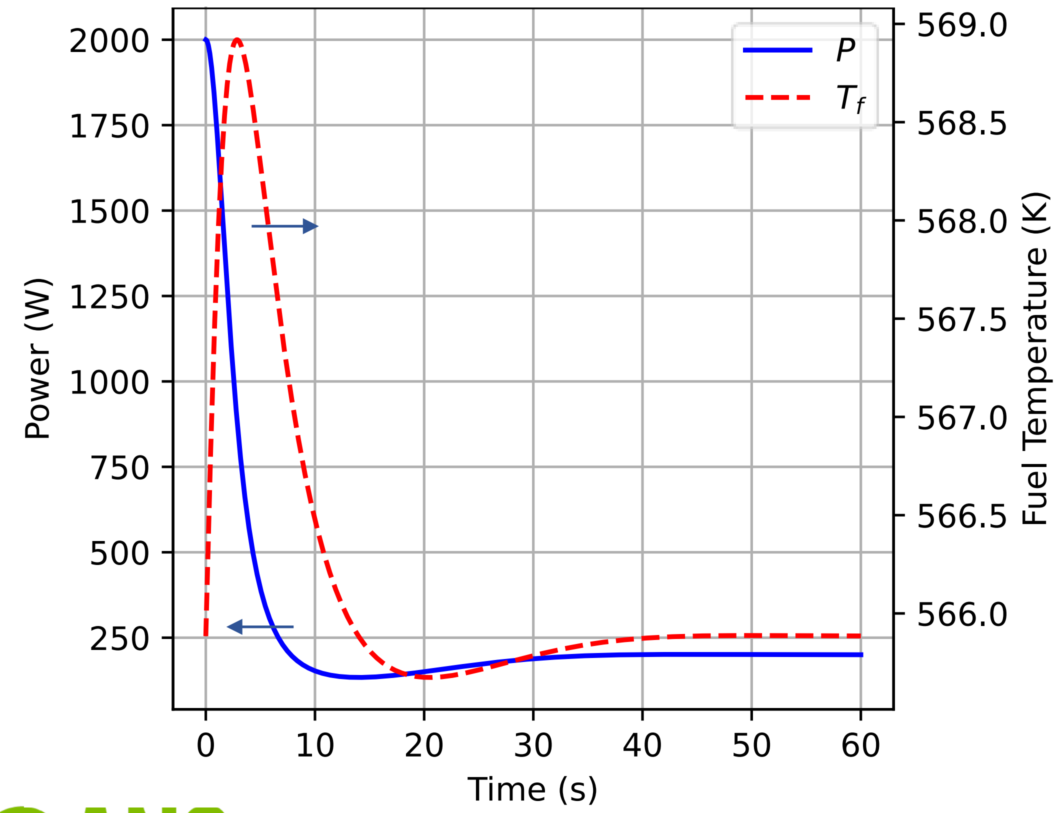
Verifying accuracy order and robustness

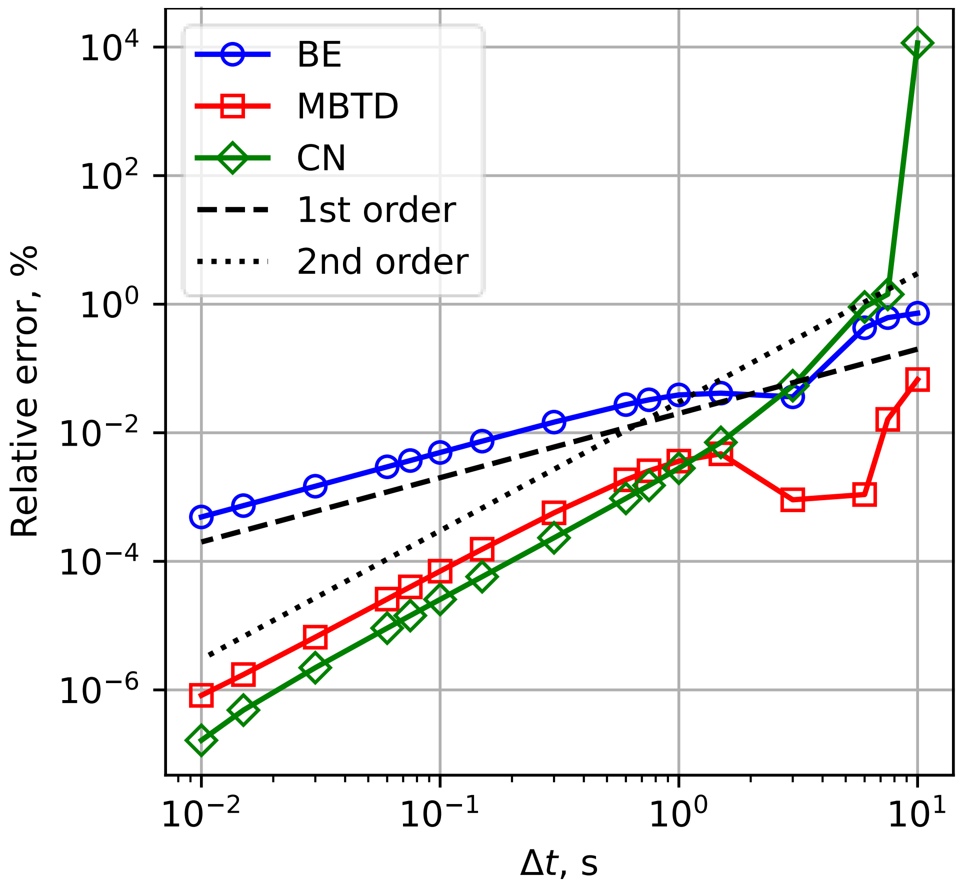
A 0D version of the test problem

- Constant T_w and $\partial\phi(t)/\partial z = \partial T_f(t)/\partial z = 0$
- Leakage cross-section Σ_L for critical IC
- Transient: $P(0^+) = 10P_{ss}$

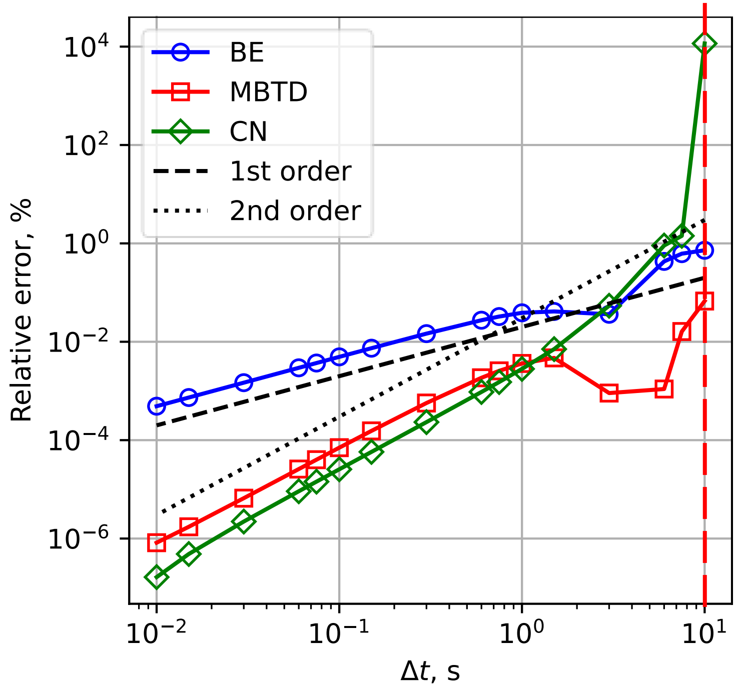
$$\frac{1}{v}\frac{d\phi}{dt} + \Sigma_L\phi(t) + \Sigma_a(T)\phi(t) = \xi\nu\Sigma_f(T)\phi(t),$$

$$\rho_f A_f Z c_{p,f}(T_f)\frac{dT_f}{dt} + 2\pi R_f Z h\left[T_f(t) - T_w\right] = q(t)$$

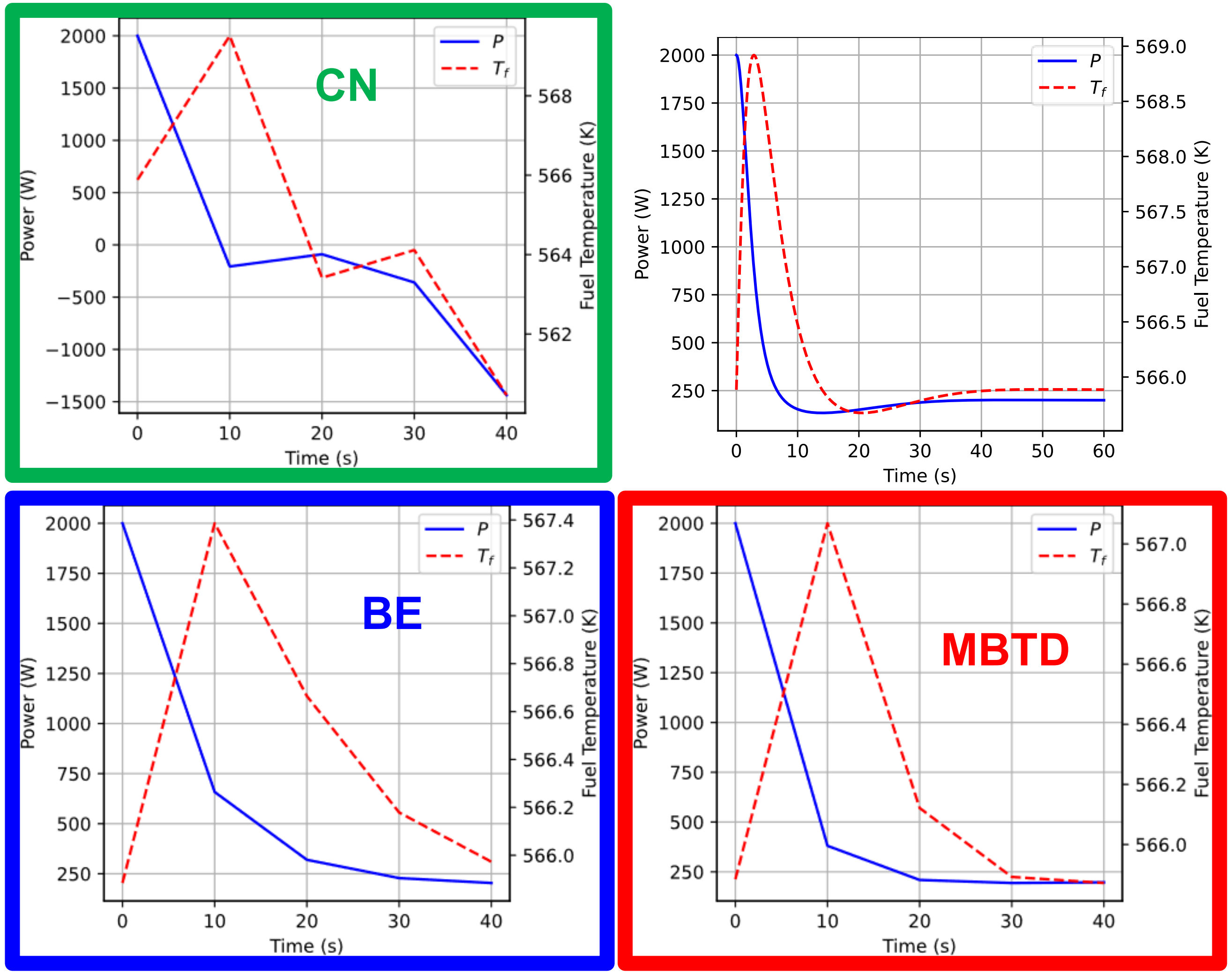




Verifying accuracy order and robustness



CN with $\Delta t = 10$ s:
- Produces negative power
- Jeopardizes feedback



Summary and future work

- MBTD is robust and 2nd-order accurate, a higher-order alternative to robust BE.
- MBTD tight-coupling technique for multi-physics problems is studied.
- Based on simplified neutronics/TH problems, MBTD is more efficient than BE for reasonably accurate simulations (total power relative error $< \sim 10\%$).
  - This generalizes earlier MBTD studies for single-physics neutronics problems.
- **Future work**
  - Testing in more practical problems (single-physics & multi-physics)
  - Improving the proposed tight-coupling (Picard Iteration) MBTD
    - Residual Balance techniques [Senecal 2018]
  - Exploring loose-coupling (Operator Splitting) techniques for MBTD
    - 2^{nd}-order Strang Splitting and Symmetrically-Weighted Sequential Splitting [MacNamara 2016]

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