Toward a Better Coupling Scheme of Co-simulation for the 1-d Conductor Model

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Motivations (1/3)

Day 2-1

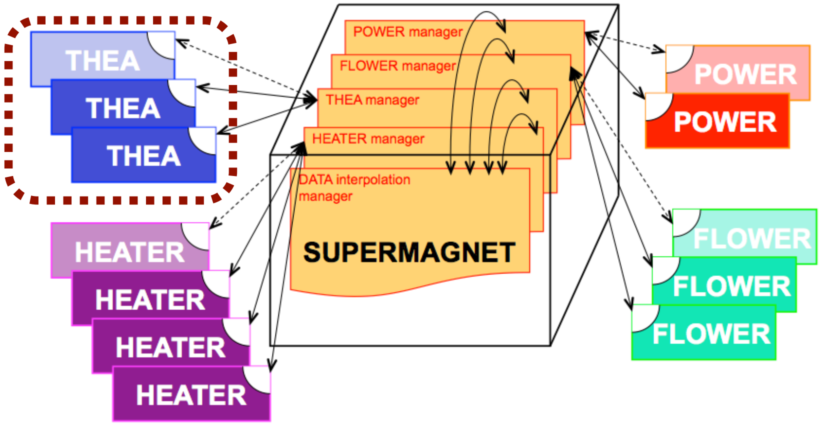
Chats 2023

Applied Superconductivity

✓ The basic idea is "binding" independent executables.

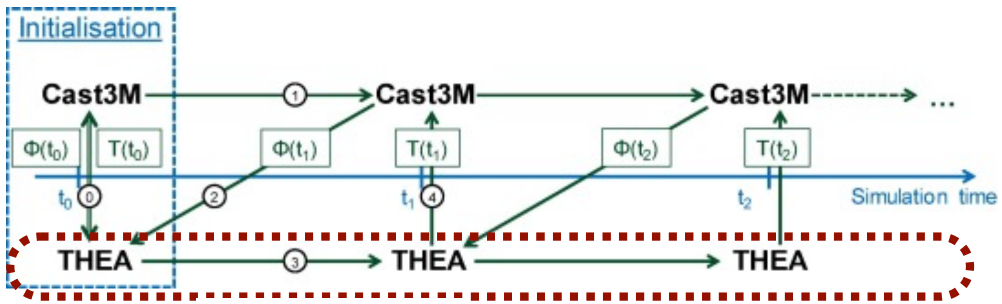
SuperMagnet : CryoSoft

THEA code



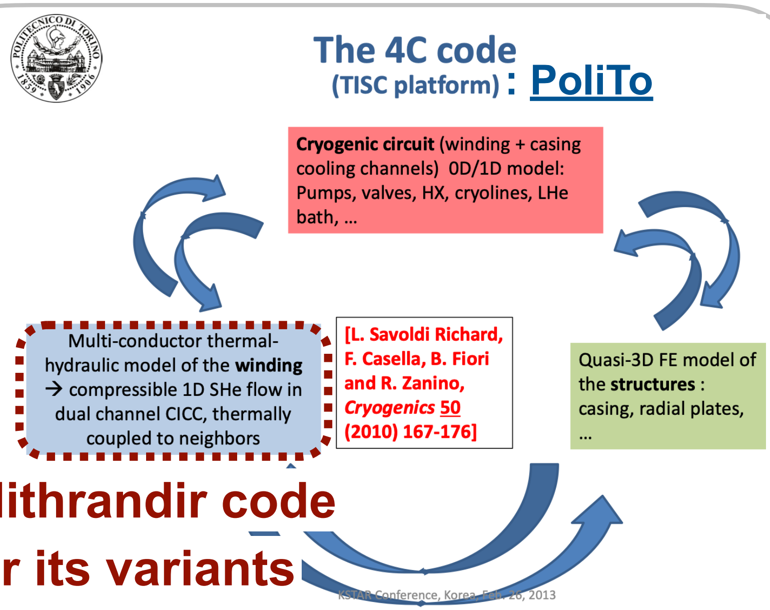
The **conductor models** are basically critical, in particular, to describe the quench behavior.

TACTICS (*THEA*-*Cast*3M-*Sim*Cryogenics) model : CEA



THEA code

The 4C code (TISC platform) : PoliTo

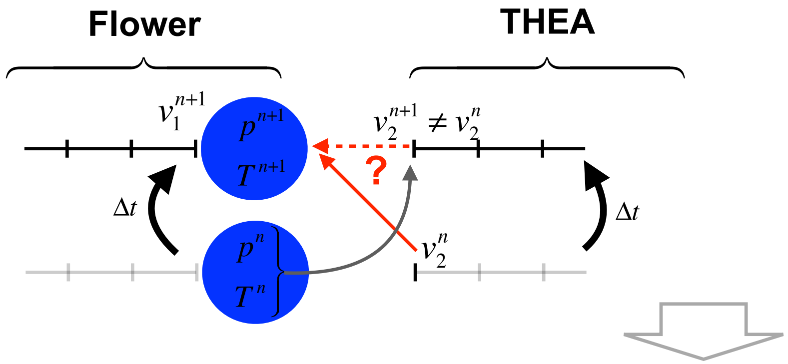


Mithrandir code or its variants

cea KFE

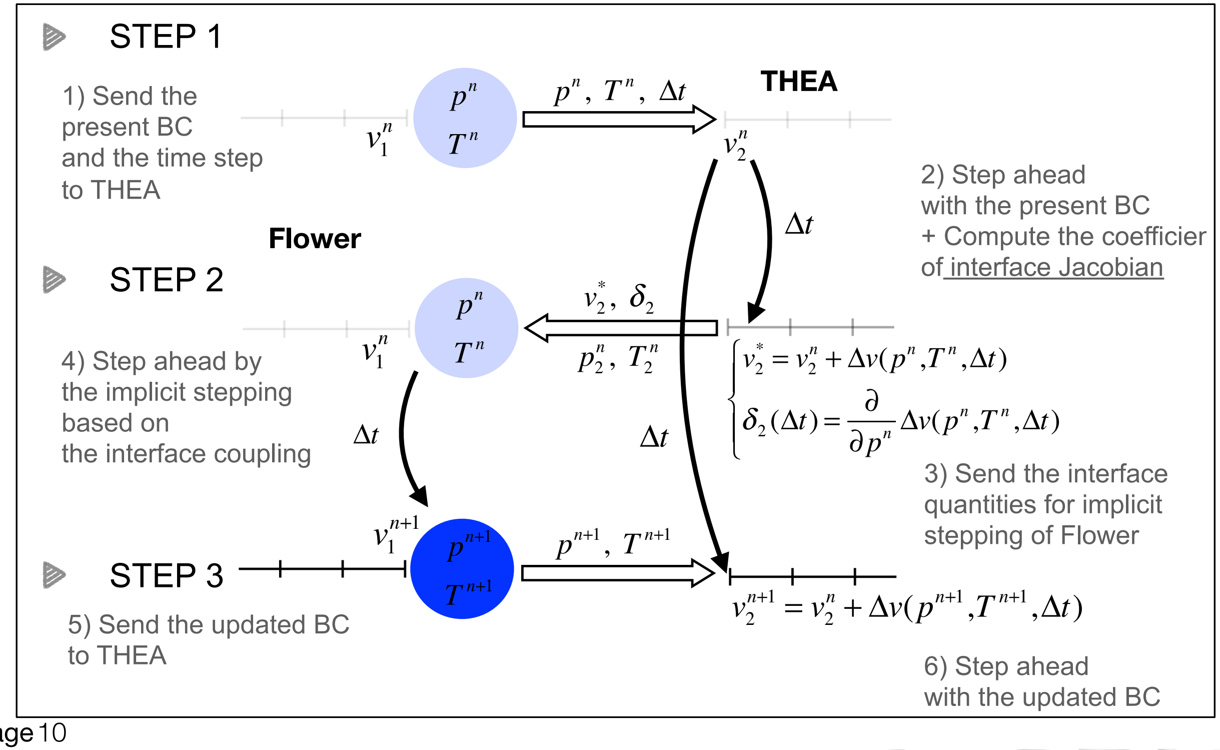
Motivations (2/3)

Issue #1 : loss of implicit coupling



✓ **Interfacial problem** is rather essential!

- To recover the implicit coupling, …

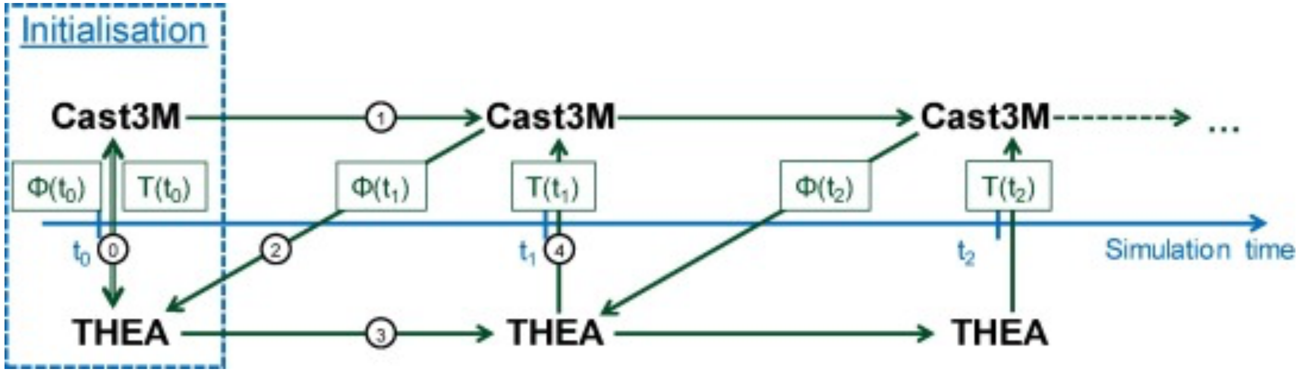


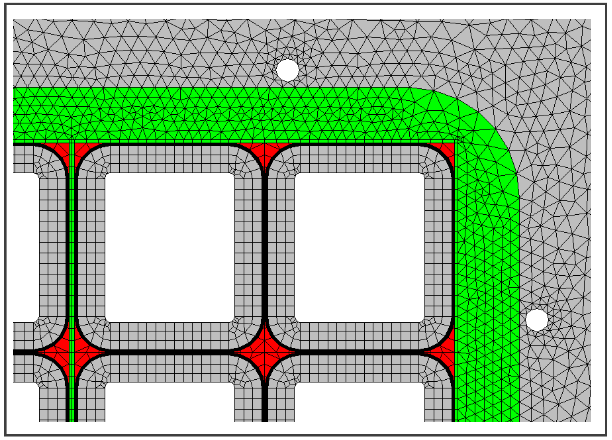
The idea is derived relying on the concept of interface Jacobian!

D. K. Oh, “[5LOrA6-08] Coupled Simulation Model of CICC Components Integrated into the Cooling Circuit” presented in ASC2019 Nov. 2 Seattle USA

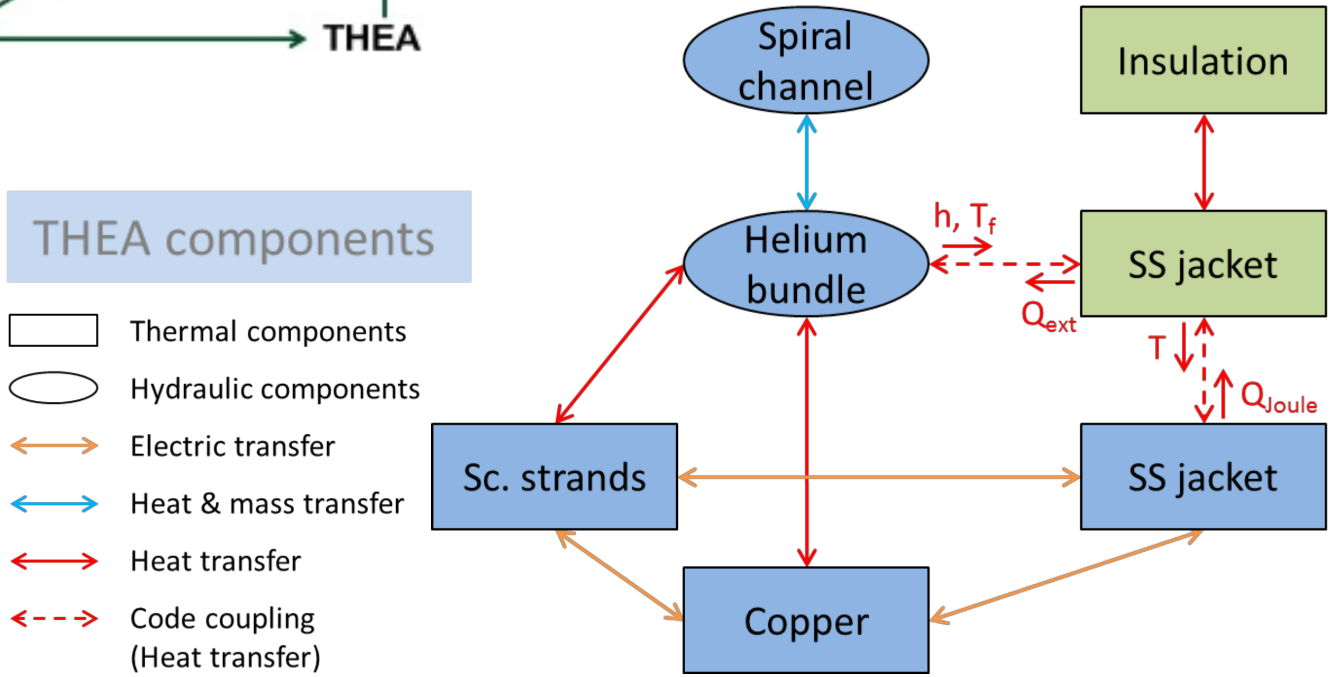
Motivations (3/3)

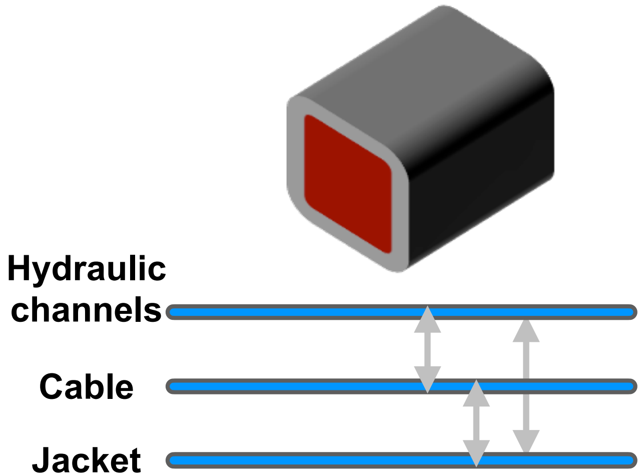
✓ Now, we are aiming at a new target i.e. the **thermal interface** of FEM meshes to a 1-d conductor model !





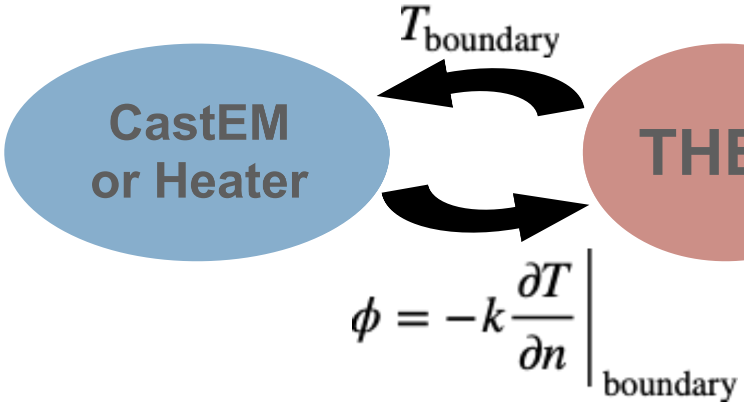
Cast3M components



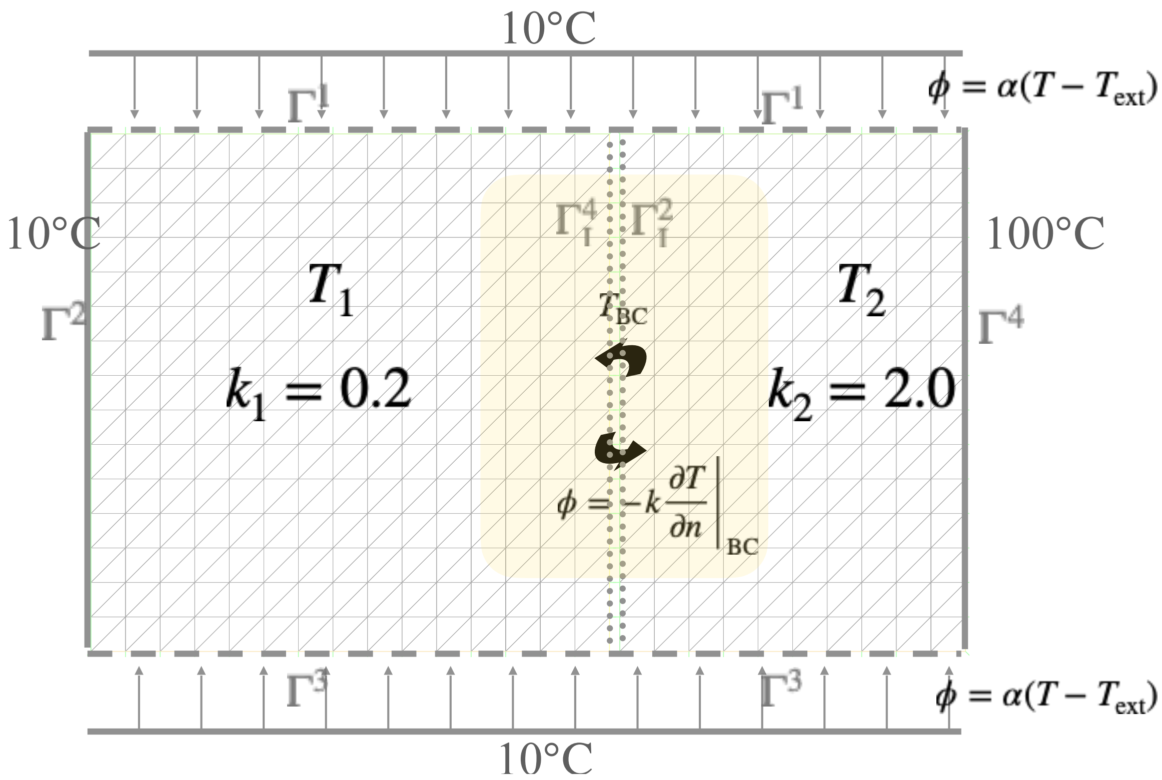


A CICC
as coupled 1-d domains

Let's make it general on the plainest consideration..



: The THEA model <u>gives the boundary temperature</u> of the solid structure (Cast3M or Heater) model, and <u>takes the heat flux</u> of the boundary.



$$\begin{cases} \dfrac{\partial T}{\partial t} - \vec{\nabla} \cdot \left(k \vec{\nabla} T \right) = q & \text{at } \Omega \\ T = T_{BC} \text{ or } \phi = -k \dfrac{\partial T}{\partial n}\Big|_{BC} & \text{at } \partial\Omega \end{cases}$$

weak form

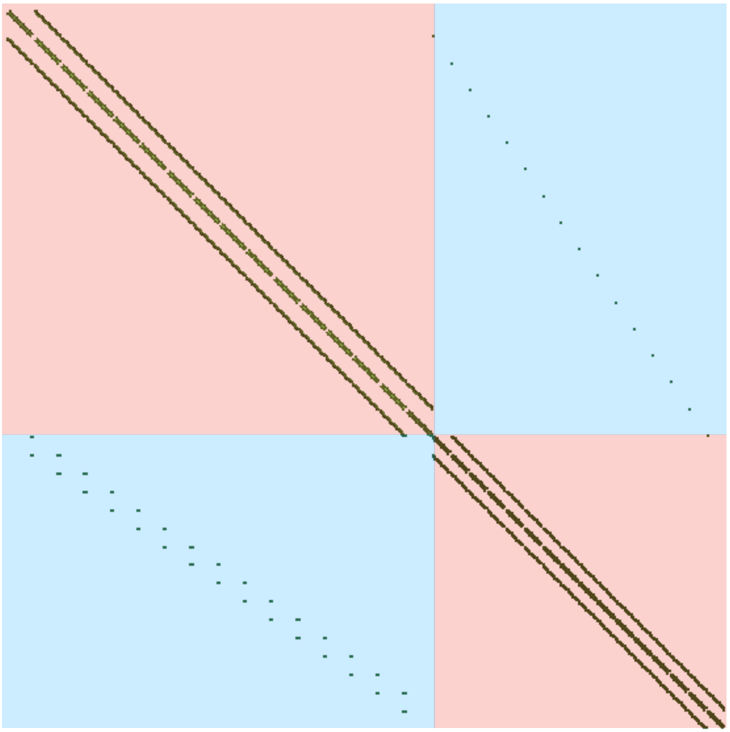
$$\int_\Omega \frac{T^{n+1} - T^n}{\Delta t} \tau \, dv + \int_\Omega k \vec{\nabla} T^{n+1} \cdot \vec{\nabla} \tau \, dv + \oint_{\partial\Omega} k \frac{\partial T^{n+1}}{\partial n} \tau \, dS = \int_\Omega q \tau \, dv$$

& boundary constraints ($T = T_{BC}$)

In the backward-Euler scheme..

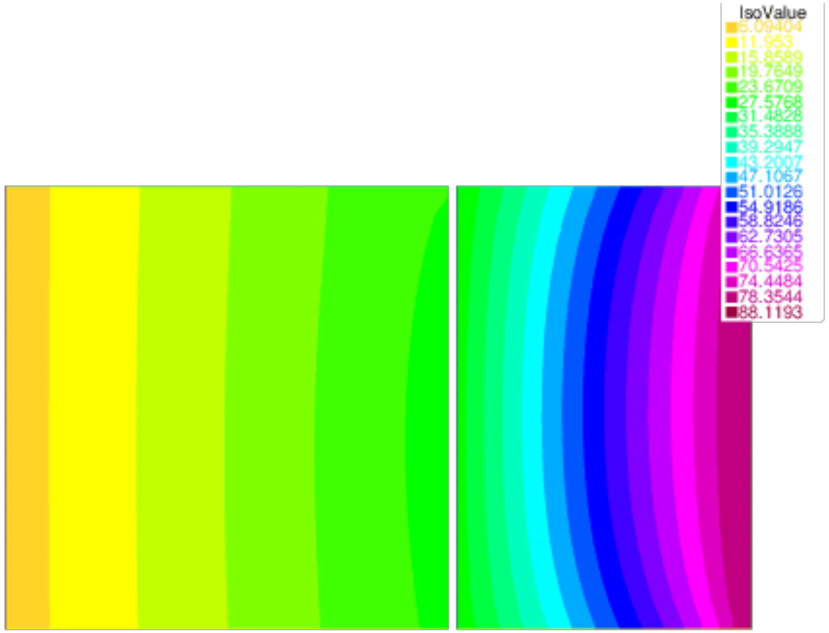
: It looks trivial, if we take them in total!

$$\begin{bmatrix} \frac{1}{\Delta t}[\mathbf{M_1}] + [\mathbf{A_1}] & [\mathbf{C_{12}}] \\ [\mathbf{C_{21}}] & \frac{1}{\Delta t}[\mathbf{M_2}] + [\mathbf{A_2}] \end{bmatrix} \cdot \begin{bmatrix} \mathbf{\Delta T_1} \\ \mathbf{\Delta T_2} \end{bmatrix} = \begin{bmatrix} \mathbf{q_1} \\ \mathbf{q_2} \end{bmatrix} - \begin{bmatrix} [\mathbf{A_1}] & [\mathbf{C_{12}}] \\ [\mathbf{C_{21}}] & [\mathbf{A_2}] \end{bmatrix} \begin{bmatrix} \mathbf{T_1^n} \\ \mathbf{T_2^n} \end{bmatrix}$$



$$T_1/\epsilon = T_2/\epsilon$$

$$-k_1 \frac{\partial T_1}{\partial n} = k_2 \frac{\partial T_2}{\partial n}$$



$t = 5 \ (\Delta t = 0.1)$

A FreeFEM++ model

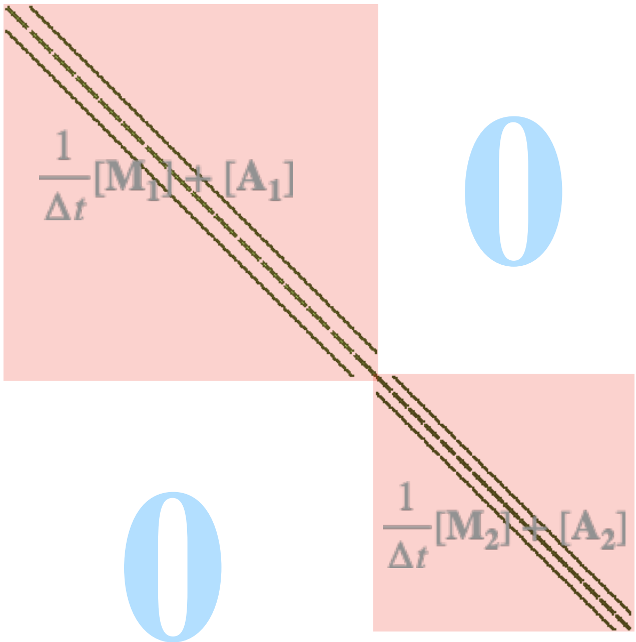
Once separated, they bring a trouble..

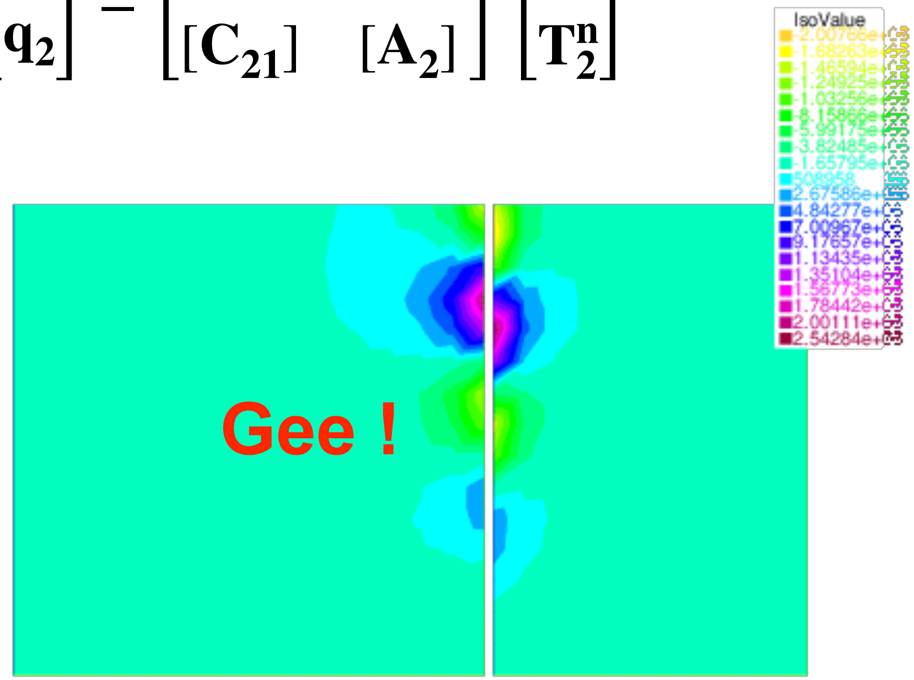
$$\begin{cases} \left(\frac{1}{\Delta t}[\mathbf{M_1}] + [\mathbf{A_1}]\right) \cdot \mathbf{\Delta T_1} = \mathbf{q_1} - [\mathbf{A_1}] \cdot \mathbf{T_1^n} - \boxed{[\mathbf{C_{12}}] \cdot \mathbf{T_2^n}} \\ \left(\frac{1}{\Delta t}[\mathbf{M_2}] + [\mathbf{A_2}]\right) \cdot \mathbf{\Delta T_2} = \mathbf{q_2} - [\mathbf{A_2}] \cdot \mathbf{T_2^n} - \boxed{[\mathbf{C_{21}}] \cdot \mathbf{T_1^n}} \end{cases}$$

Setting T_{BC} to #1

Transferring $-k\left.\frac{\partial T}{\partial n}\right|_{BC}$ to #2

$$\begin{bmatrix} \frac{1}{\Delta t}[\mathbf{M_1}] + [\mathbf{A_1}] & \mathbf{0} \\ \mathbf{0} & \frac{1}{\Delta t}[\mathbf{M_2}] + [\mathbf{A_2}] \end{bmatrix} \cdot \begin{bmatrix} \mathbf{\Delta T_1} \\ \mathbf{\Delta T_2} \end{bmatrix} = \begin{bmatrix} \mathbf{q_1} \\ \mathbf{q_2} \end{bmatrix} - \begin{bmatrix} [\mathbf{A_1}] & [\mathbf{C_{12}}] \\ [\mathbf{C_{21}}] & [\mathbf{A_2}] \end{bmatrix} \begin{bmatrix} \mathbf{T_1^n} \\ \mathbf{T_2^n} \end{bmatrix}$$





$t = 5\ (\Delta t = 0.1)$

How to recover the lost terms

In sequence

$$\Delta \mathbf{T}_1^* = \left(\frac{1}{\Delta t}[\mathbf{M}_1] + [\mathbf{A}_1]\right)^{-1} \cdot \left(\mathbf{q}_1 - [\mathbf{A}_1]\cdot \mathbf{T}_1^n - [\mathbf{C}_{12}]\cdot \mathbf{T}_2^n\right)$$

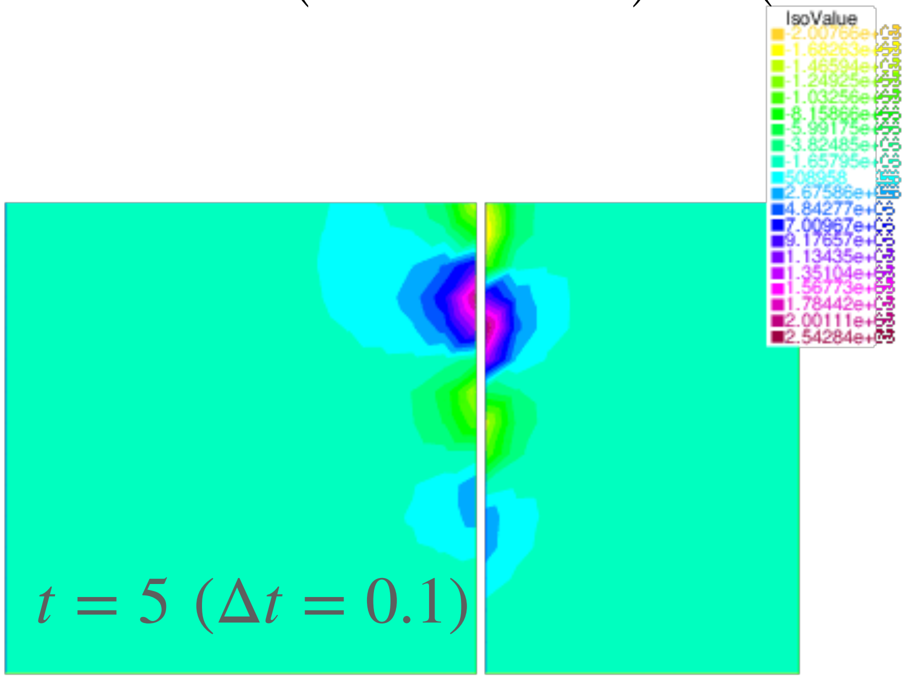
trial solution

$$\Delta \mathbf{T}_2 = \left(\frac{1}{\Delta t}[\mathbf{M}_2] + [\mathbf{A}_2] - \boxed{[\mathbf{C}_{21}]\cdot[\bar{\mathbf{C}}_{12}]}\right)^{-1} \cdot \left(\mathbf{q}_2 - [\mathbf{A}_2]\cdot \mathbf{T}_2^n - [\mathbf{C}_{21}]\cdot \boxed{\left(\mathbf{T}_1^n + \Delta \mathbf{T}_1^*\right)}\right)$$

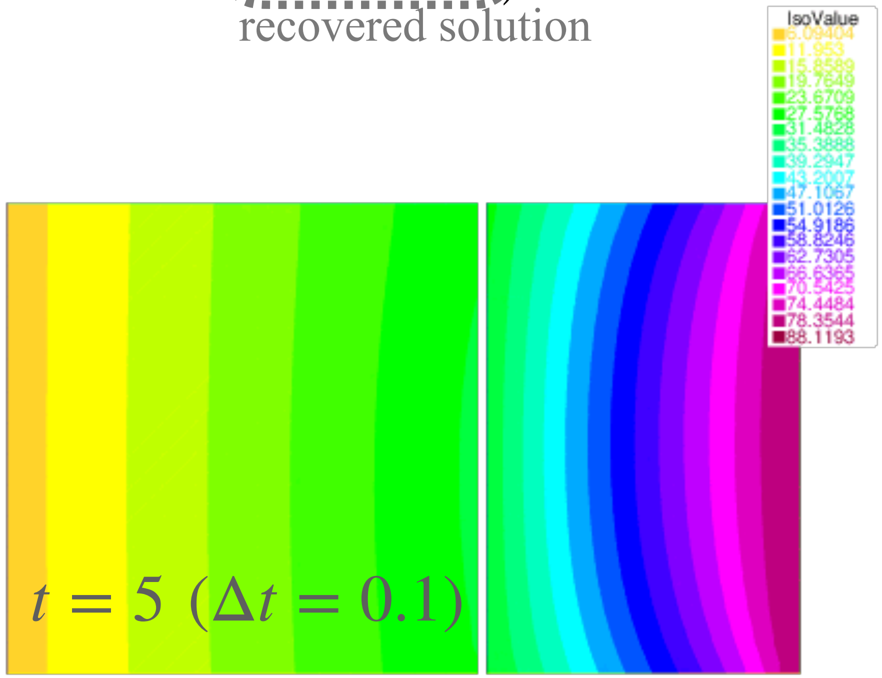
interface Jacobian

$$\Delta \mathbf{T}_1 = \left(\frac{1}{\Delta t}[\mathbf{M}_1] + [\mathbf{A}_1]\right)^{-1} \cdot \left(\mathbf{q}_1 - [\mathbf{A}_1]\cdot \mathbf{T}_1^n - [\mathbf{C}_{12}]\cdot \boxed{\left(\mathbf{T}_2^n + \Delta \mathbf{T}_2\right)}\right)$$

recovered solution



Without IJ



With IJ

The interface Jacobian makes implicit steps true!

A Lesson Learned

: Conceptually, the interface Jacobian means **changing rate of the boundary value** with respect to the upcoming solution!

➡ However, the changing rate is just **one**, naturally implicated by the fixed BC for #1

$$[\mathbf{C}_{21}] \cdot \boxed{[\bar{\mathbf{C}}_{12}]} \cdot \Delta \mathbf{T}_2$$

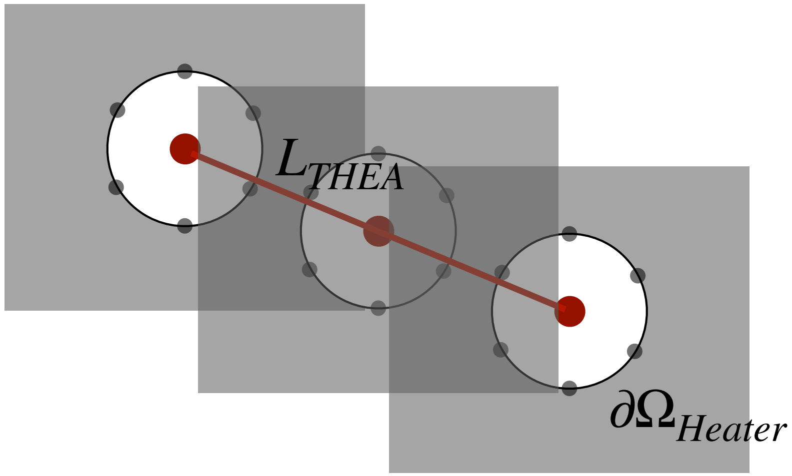
Along the boundary,
it just maps the nodal indices of #2
to the indices of #1

The FEM matrix of boundary heat flux
as the integration over shape functions along the boundary

$$: \int_{\partial\Omega} -k \frac{\partial T^{n+1}}{\partial n} \tau \, dS \longrightarrow \sum_{ij} \left\{ \int_{\partial\Omega} -k \frac{\partial w_i}{\partial n} v_j \, dS \right\} T_{1i} T_{2j}$$

➡ So, the point is transferring the coefficients of heat flux to the THEA model to build a new component of the system matrix.

For our <u>actual target</u>, i.e., of THEA-Cast3M, or THEA-Heater coupling..



$$q_{THEA} = -\oint_{\partial\Omega_{Heater}} k \frac{\partial T}{\partial n}\, dS$$

☞ **So, the coupling matrix [C_{21}] can be derived from the integral over $\partial\Omega_{Heater}$ and L_{THEA}**

i.e. $\displaystyle\int_{L_{THEA}} \oint_{\partial\Omega_{Heater}} -k \frac{\partial w_i(S,x)}{\partial n}\, dS\; v_j(x)\, dx$.

☞ Actually, the interface Jacobian terms are represented simply as the rate $\mathbf{\Delta Q/\Delta T}$, i.e., how much the heat load will vary, if the boundary temperature is changed.

<u>So, we revise the THEA code to consider such an idea..</u>

Let's revise the THEA code..

$$\left\{ \frac{[\mathbf{M}]}{\Delta t} + \big([\mathbf{A}] + [\mathbf{G}] - [\mathbf{S}]\big) \right\} \cdot \mathbf{\Delta U} = \mathbf{Q} - \big([\mathbf{A}] + [\mathbf{G}] - [\mathbf{S}]\big) \cdot \mathbf{U}^n$$

$$\mathbf{Q} = \mathbf{Q}^n + [\mathbf{C}] \cdot \Delta\mathbf{T}_{\mathrm{bc}} \longleftarrow \quad [\mathbf{C}] = \left[\int_L w_i^{\mathrm{T}} \boxed{\left(\frac{\Delta q_i}{\Delta T_j} \right)_{\text{per BC DoF}}} w_j \, dx \right]$$

☞ Actually, $\left(\frac{\Delta q_i}{\Delta T_j} \right)$ is <u>diagonal</u>.

$$\boxed{\left\{ \frac{[\mathbf{M}]}{\Delta t} + \big([\mathbf{A}] + [\mathbf{G}] - [\mathbf{S}] - \boxed{[\mathbf{C}]}\big) \right\} \cdot \mathbf{\Delta U} = \mathbf{Q}^n - \big([\mathbf{A}] + [\mathbf{G}] - [\mathbf{S}]\big) \cdot \mathbf{U}^n}$$

<u>That's it!</u>

: The THEA code is now revised in consistent with our idea to include the IJ terms.

What about the counter parts of THEA?

: **We are looking for <u>high level commands</u> to evaluate the coupling matrix (or the integral of shape functions).**

CHAP. 2.1: STATIONARY LINEAR THERMAL ANALYSIS
CONVECTION AND VOLUME HEAT SOURCE

- Mathematical formulation

```
* CONVECTION MODEL
MOC       = MODE LHAUT 'THERMIQUE' 'CONVECTION' ;
MAC       = MATE MOC 'H' 100. ;
```

- Conductivity matrix (but for convection !)

```
* FIRST MEMBER FOR CONVECTION
CONH      = COND MOC MAC ;
```

$$[K] = \int_V [B]^T[\lambda][B]dV + \int_{\partial V\varphi} h[N]^T[N]dS$$

- Equivalent nodal heat flux vector (convection)

```
* SECOND MEMBER FOR CONVECTION
CHTC      = MANU 'CHPO' LHAUT 'T' T0 ;
FLH       = CONV MOC MAC CHTC ;
```

$$\{F\} = \int_V [N]^T q\, dV + \int_{\partial V\varphi} [N]^T \left(\varphi_{imp} + hT_f + \varepsilon\sigma(T_\infty^4 - T^4)\right) dS$$

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$$\boxed{[\mathbf{C}_{21}]} \cdot [\bar{\mathbf{C}}_{12}] \cdot \mathbf{\Delta T}_2 \longrightarrow$$

$$\int_L dx \boxed{\int_{\partial\Omega} -k\frac{\partial w_i}{\partial n}\, dS}$$

$$\longrightarrow \left.\frac{\mathbf{\Delta Q}_1}{\mathbf{\Delta T}_2}\right|_{\text{per BC}}$$

http://www-cast3m.cea.fr/html/formations/Starting_with_Cast3M.pdf

Regarding the Heater code,..

: The Heater code, like all the CryoSoft codes, solves the equations with constraints (fixed boundaries), computing their residuals on the r.h.s..

to be solved | fixed | fixed

$$[\mathbf{F}]\begin{bmatrix}\mathbf{T}_1^{\,n+1}-\mathbf{T}_1^{\,n}\\ \mathbf{T}_2^{\,n+1}-\mathbf{T}_2^{\,n}\end{bmatrix} = \begin{bmatrix}\mathbf{Q}_1\\ \mathbf{Q}_2\end{bmatrix} - \left([\mathbf{A}]+[\mathbf{G}]-[\mathbf{S}]\right)\begin{bmatrix}\mathbf{T}_1^{\,n}\\ \mathbf{T}_2^{\,n}\end{bmatrix}$$

constraint (fixed) | residual (to be solved)

1 : core
2 : boundary

Where $[\mathbf{F}] = \dfrac{[\mathbf{M}]}{\Delta t} + \left([\mathbf{A}]+[\mathbf{G}]-[\mathbf{S}]\right)$

☞ We are better to change the solution scheme for correct evaluation of the IJ terms.

to be solved | fixed | fixed

$$[\mathbf{F}]\begin{bmatrix}\mathbf{T}_1^{\,n+1}-\mathbf{T}_1^{\,n}\\ \mathbf{0}\end{bmatrix} = \begin{bmatrix}\mathbf{Q}_1\\ \mathbf{Q}_2\end{bmatrix} - \left([\mathbf{A}]+[\mathbf{G}]-[\mathbf{S}]\right)\begin{bmatrix}\mathbf{T}_1^{\,n}\\ \mathbf{T}_2^{\,n+1}\end{bmatrix}$$

residual (to be solved) | constraint (fixed)

Let's revise the Heater code..

: Then, the IJ terms are obtained as the variation along with the boundary temperatures.

solution (dummy)

$$[\mathbf{F}]\begin{bmatrix}\boldsymbol{\Delta T'}\\ \mathbf{0}\end{bmatrix} = \begin{bmatrix}\mathbf{0}\\ \dfrac{\boldsymbol{\Delta Q}}{\boldsymbol{\Delta T}}\end{bmatrix} - \left([\mathbf{A}] + [\mathbf{G}] - [\mathbf{S}]\right)\begin{bmatrix}\mathbf{0}\\ \mathbf{1}\end{bmatrix} \begin{array}{l} : \ \text{core} \\ : \ \text{boundary}\end{array}$$

residual (what we need)

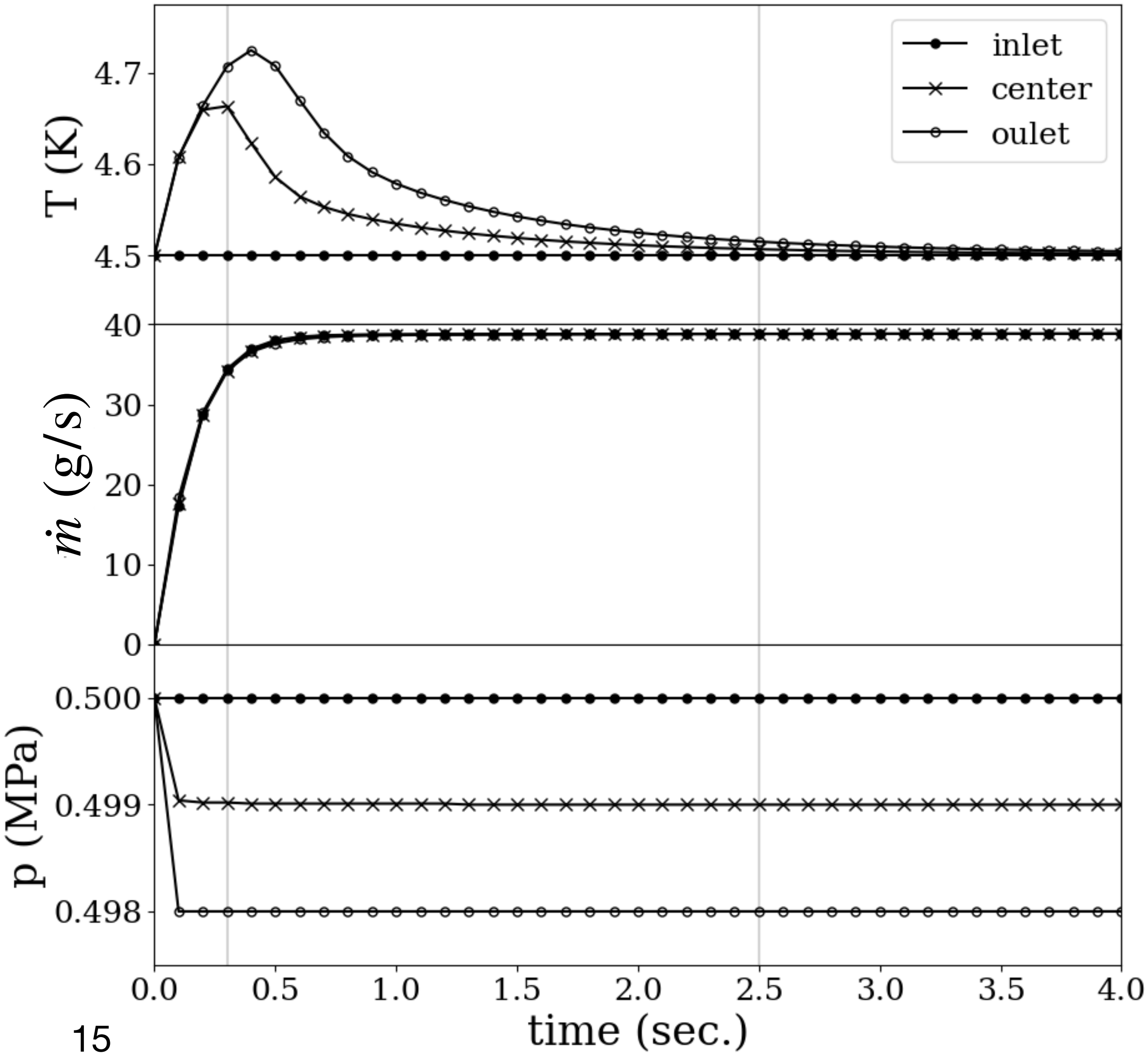
☞ That means we need to solve the matrix again to obtain the IJ terms of $\dfrac{\boldsymbol{\Delta Q}}{\boldsymbol{\Delta T}}$, which looks costful; any cheaper approximation?

☞ The Heater code is <u>updated to evaluate the additional terms of IJ</u> which will be transferred to the THEA code to compose the $[\mathbf{C}]$-matrix

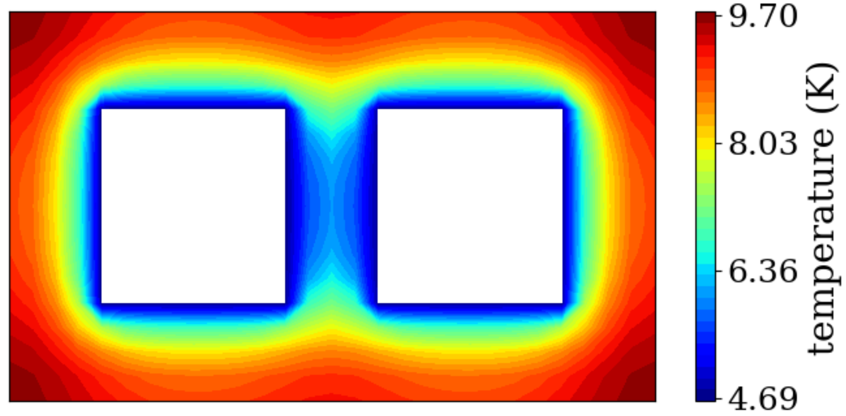
Verification (1/4)

: Let's consider a co-current SUS304 heat exchanger, initially at 10K, with two helium channels (1m) of rectangular flow area (1cm x 1cm)..

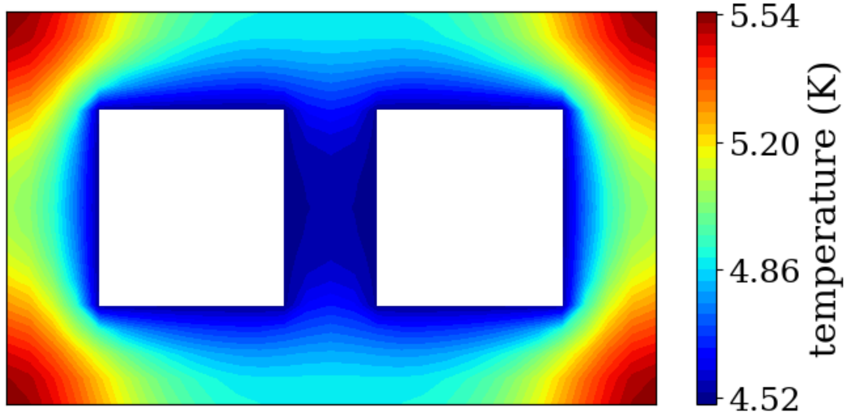
- **hydraulic flows**



- **outlet temperature**



time = 0.3 sec.

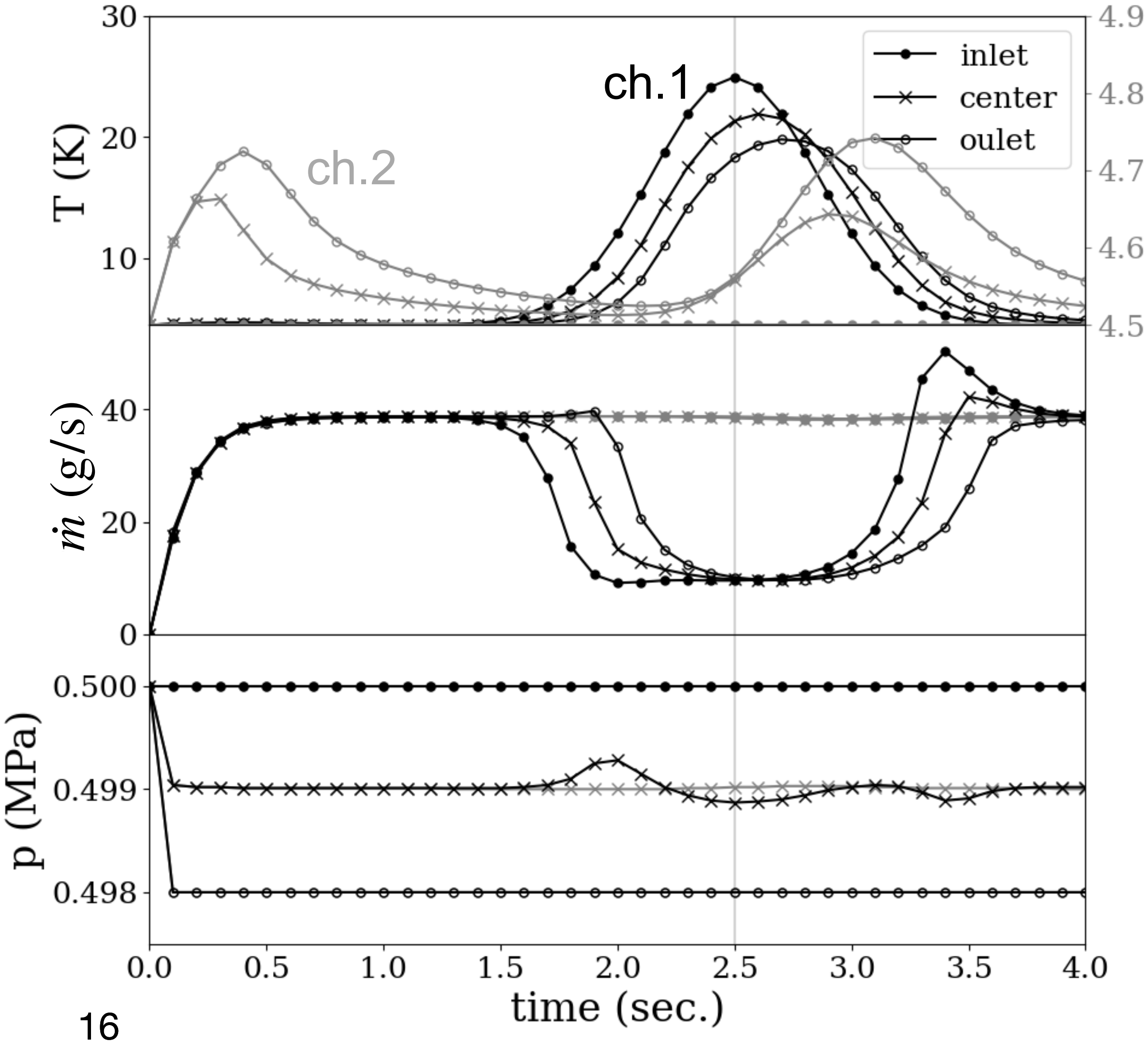


time = 2.5 sec.

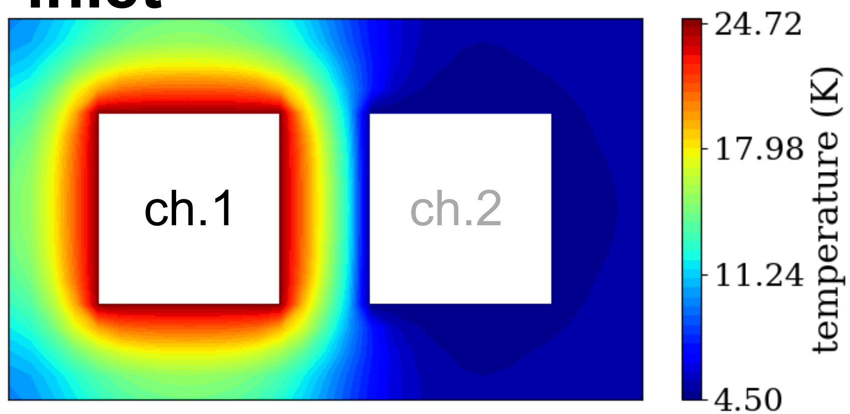
Verification (2/4)

: Then, let's change the inlet temperature
of the channel 1 up to 25K and more around 2.5 sec.

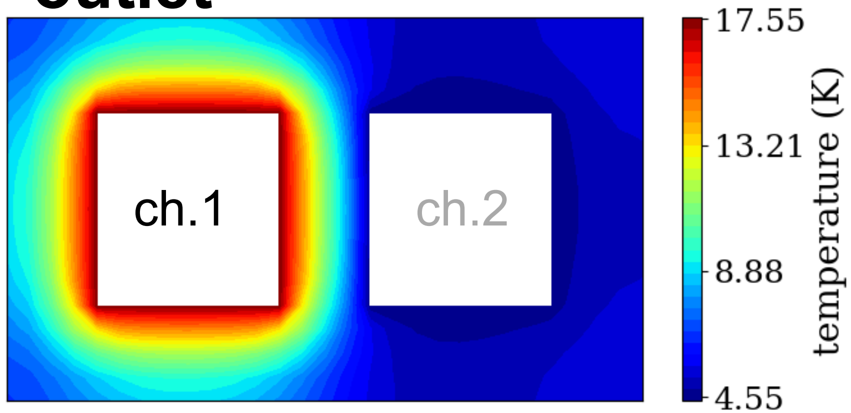
- **hydraulic flows**



- **inlet**



- **outlet**



time = 2.5 sec.

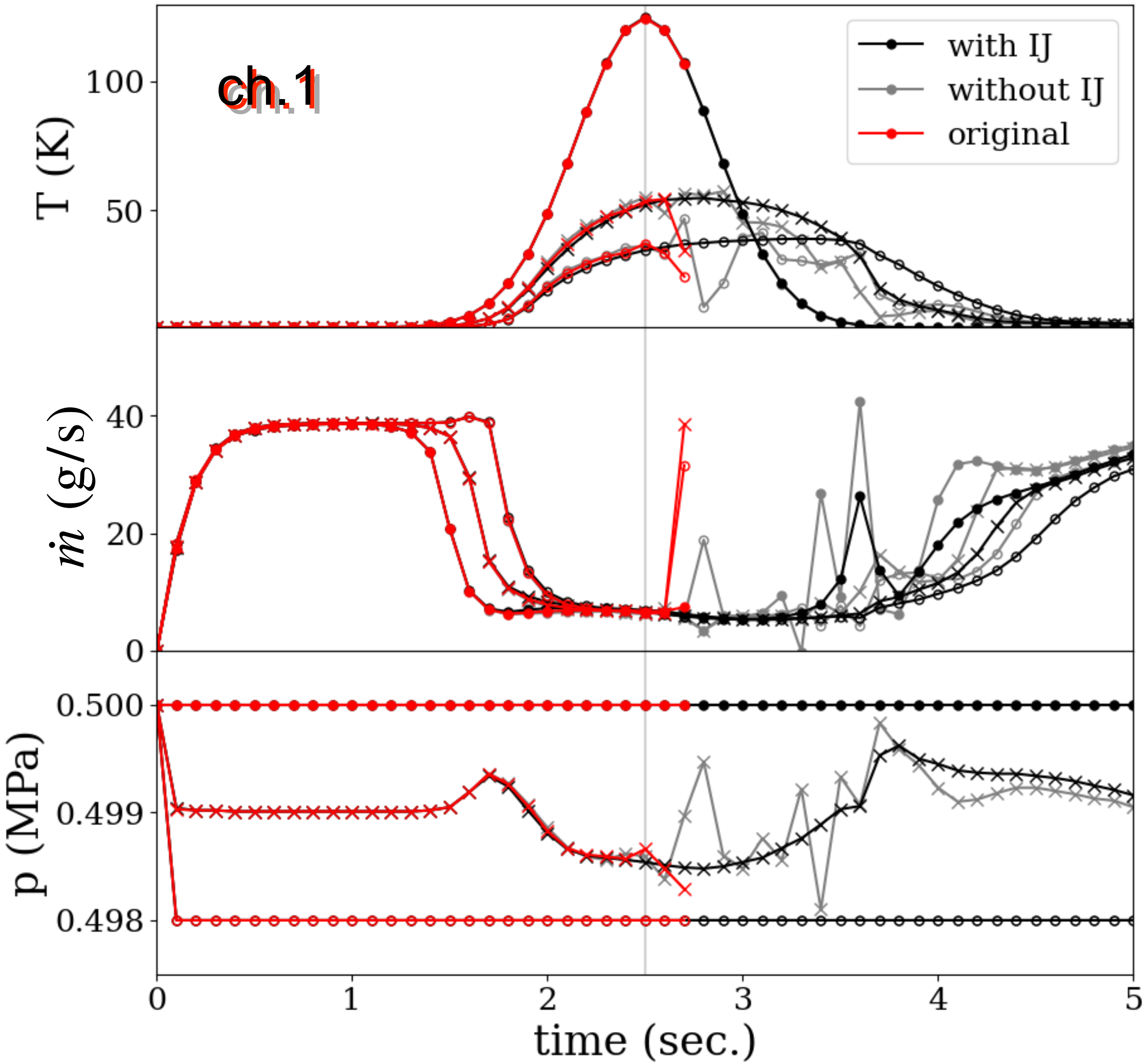
Verification (3/4)

: What about the stability? ➡ CPU time can be an indicator.

T_{peak} (K)	**Original** (CPU time in sec.)	**Modified** (CPU time in sec.)	
		Without IJ	**With IJ**
50	**13.6** (H1) 0.59 (T1) 0.61 (T2)	**10.2** (H1) 0.57 (T1) 0.59 (T2)	**10.5** (H1) 0.57 (T1) 0.62 (T2)
75	**16.7** (H1) 0.61 (T1) 0.60 (T2)	**10.5** (H1) 0.56 (T1) 0.59 (T2)	**10.5** (H1) 0.56 (T1) 0.61 (T2)
100	**17.9** (H1) 1.17 (T1) 0.60 (T2)	**10.3** (H1) 0.63 (T1) 0.57 (T2)	**10.4** (H1) 0.57 (T1) 0.60 (T2)
125	**broken solution** (at ~60% eval.)	**11.8** (H1) 1.40 (T1) 0.60 (T2)	**10.5** (H1) 0.65 (T1) 0.59 (T2)

Verification (4/4)

: Let's look into the case of inlet temperature 125 K.



Improved, but..

➡ The hydraulic terminals seem to be the source of instability!

Conclusion

- **A better coupling scheme for integrated modeling is introduced on the lesson learned from the plainest case of thermal contact.**

☞ The issue of THEA-Cast3M models in quench is to be understood by pointing out the source of trouble on our attempt of new coupling scheme.

Supplements

Issue #2 : hard boundary constraints

We already developed such a boundary scheme..

* We applied them to the CICC (THEA) models..

Inlet :

$$\begin{cases} [\mathbf{AU}]_{v,\, i=1} = \bar{v}\left(\frac{v_2 - v_1}{2}\right) + \frac{1}{\bar{\rho}}\left(\frac{p_2 - p_0^{(\mathrm{in})}}{2}\right) + \frac{\bar{v}}{\bar{\rho}\bar{c}}\left(\frac{p_1 - p_0^{(\mathrm{in})}}{2}\right) \\ [\mathbf{AU}]_{p,\, i=1} = \bar{\rho}\bar{c}^2\left(\frac{v_2 - v_1}{2}\right) + \bar{v}\left(\frac{p_2 - p_0^{(\mathrm{in})}}{2}\right) + \boxed{\bar{c}\left(\frac{p_1 - p_0^{(\mathrm{in})}}{2}\right)} \\ [\mathbf{AU}]_{T,\, i=1} = \overline{\rho\phi C_v T}\left(\frac{v_2 - v_1}{2}\right) + \boxed{\overline{\rho C_v v}\left(\frac{T_2 + T_1}{2} - T_0^{(\mathrm{in})*}\right)} + \frac{\overline{\phi C_v T}(\bar{c} - \bar{v})}{\bar{c}^2}\left(\frac{p_1 - p_0^{(\mathrm{in})}}{2}\right) \end{cases}$$

Negligible

The boundary pressure follows the constraint in the speed of sound.

The boundary temperature follows the upwind constraint in the flow velocity.

Outlet :

$$\begin{cases} [\mathbf{AU}]_{v,\, i=\mathrm{n}} = \bar{v}\left(\frac{v_\mathrm{n} - v_{\mathrm{n}\text{-}1}}{2}\right) + \frac{1}{\bar{\rho}}\left(\frac{p_0^{(\mathrm{out})} - p_{\mathrm{n}\text{-}1}}{2}\right) + \frac{\bar{v}}{\bar{\rho}\bar{c}}\left(\frac{p_\mathrm{n} - p_0^{(\mathrm{out})}}{2}\right) \\ [\mathbf{AU}]_{p,\, i=\mathrm{n}} = \bar{\rho}\bar{c}^2\left(\frac{v_\mathrm{n} - v_{\mathrm{n}\text{-}1}}{2}\right) + \bar{v}\left(\frac{p_0^{(\mathrm{out})} - p_{\mathrm{n}\text{-}1}}{2}\right) + \boxed{\bar{c}\left(\frac{p_\mathrm{n} - p_0^{(\mathrm{out})}}{2}\right)} \\ [\mathbf{AU}]_{T,\, i=\mathrm{n}} = \overline{\rho\phi C_v T}\left(\frac{v_\mathrm{n} - v_{\mathrm{n}\text{-}1}}{2}\right) + \boxed{\overline{\rho C_v v}\left(T_0^{(\mathrm{out})*} - \frac{T_{\mathrm{n}\text{-}1} + T_\mathrm{n}}{2}\right)} + \frac{\overline{\phi C_v T}(\bar{c} - \bar{v})}{\bar{c}^2}\left(\frac{p_\mathrm{n} - p_0^{(\mathrm{out})}}{2}\right) \end{cases}$$

An application of the decomposed flux boundary (Eq 4 and Eq 5) in the reference, *i.e.*,
D. K. Oh and S. Oh, “Improved 1-d hydraulic network model for cryogenic circuits coupled to CICC models of fusion magnet systems” *Cryogenics 97 (2019) 133-143*

Actually, there is a trick.

$$[\mathbf{IJ}] = [\mathbf{C}_{21}] \cdot \left(\frac{1}{\Delta t}[\mathbf{M}_1] + [\mathbf{A}_1] \right)^{-1} \cdot [\mathbf{C}_{12}]$$

At a glance, matrix inversion seems not avoidable!

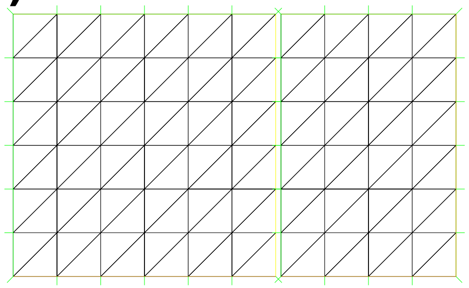
Nonetheless, don't forget the artificial elements (TGV) assigned to be LARGE enough, typically, as 10^{30} to impose the static constraint of temperature boundary condition.

$$\text{Let} \quad [\bar{\mathbf{C}}_{12}] = 10^{-30} \times [\mathbf{C}_{12}] \quad \Rightarrow \quad \left(\frac{1}{\Delta t}[\mathbf{M}_1] + [\mathbf{A}_1] \right) \cdot [\bar{\mathbf{C}}_{12}] \approx [\mathbf{C}_{12}]$$

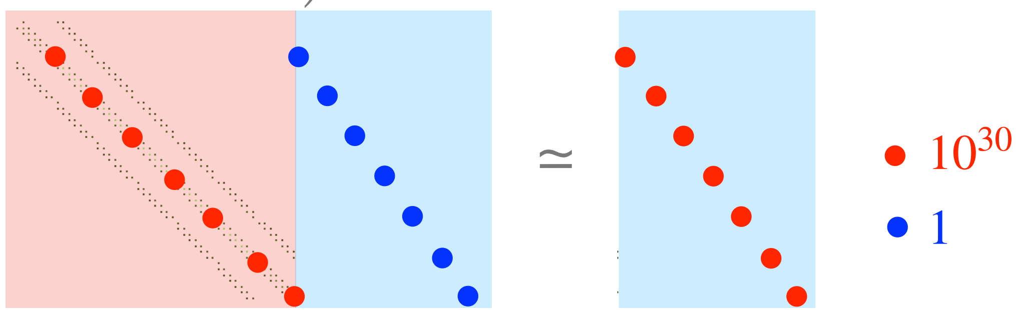
This means $[\bar{\mathbf{C}}_{12}]$ has the same structure with elements of 1 instead of 10^{30} !

$$[\mathbf{IJ}] \approx [\mathbf{C}_{21}] \cdot [\bar{\mathbf{C}}_{12}]$$

Ex)



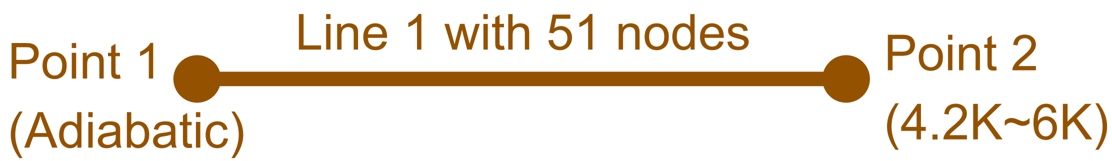
$$\left(\frac{1}{\Delta t}[\mathbf{M}_1] + [\mathbf{A}_1] \right) \cdot [\bar{\mathbf{C}}_{12}] \approx [\mathbf{C}_{12}]$$

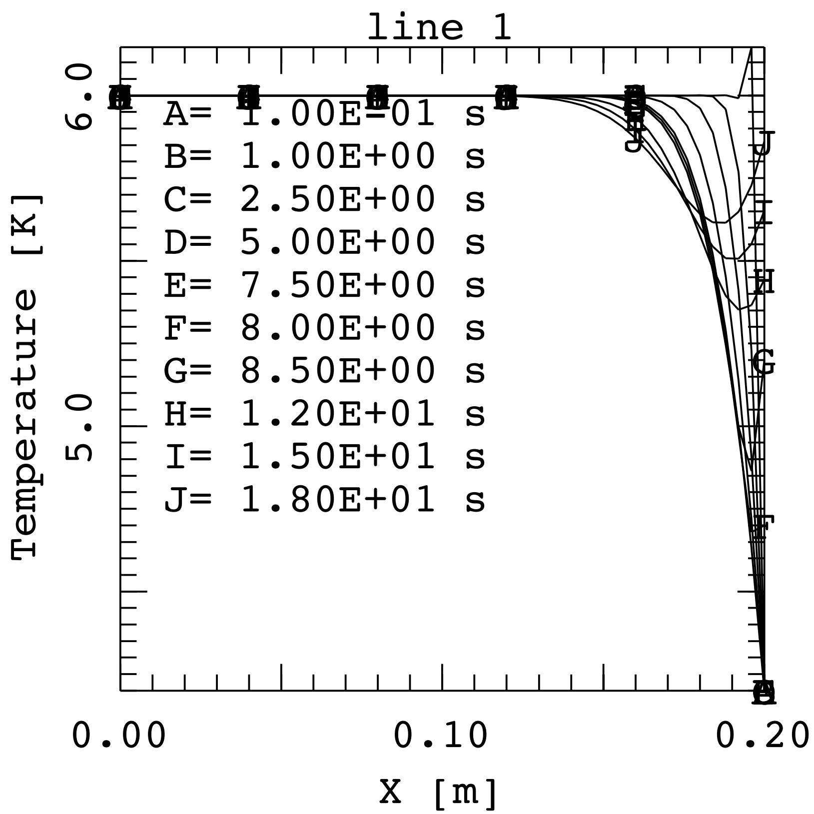


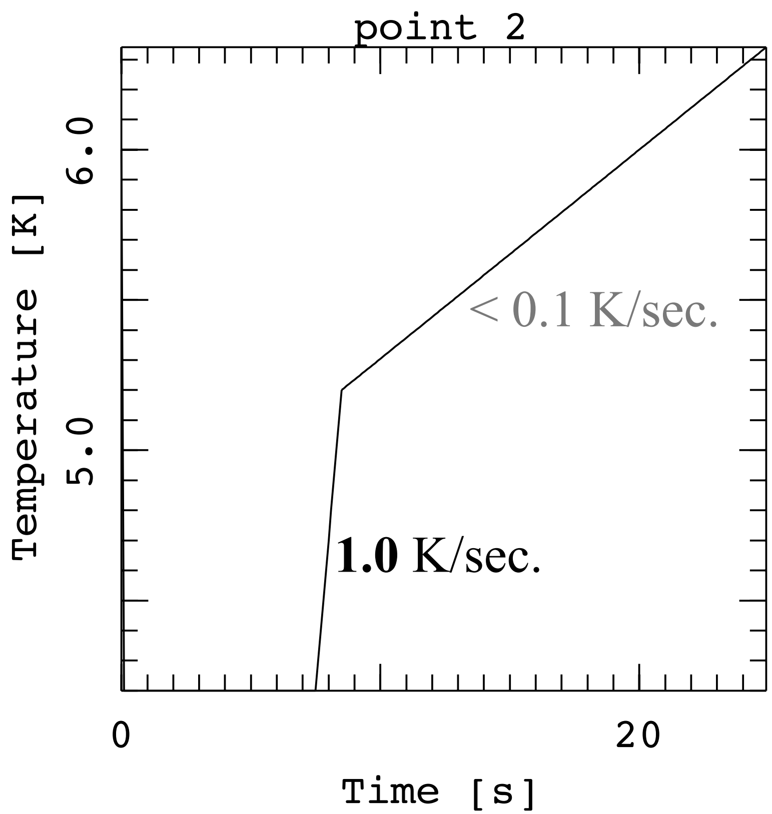
Solution scheme.. What? (1/2)

Let's check the simple 1-d Heater model of a metal wire:

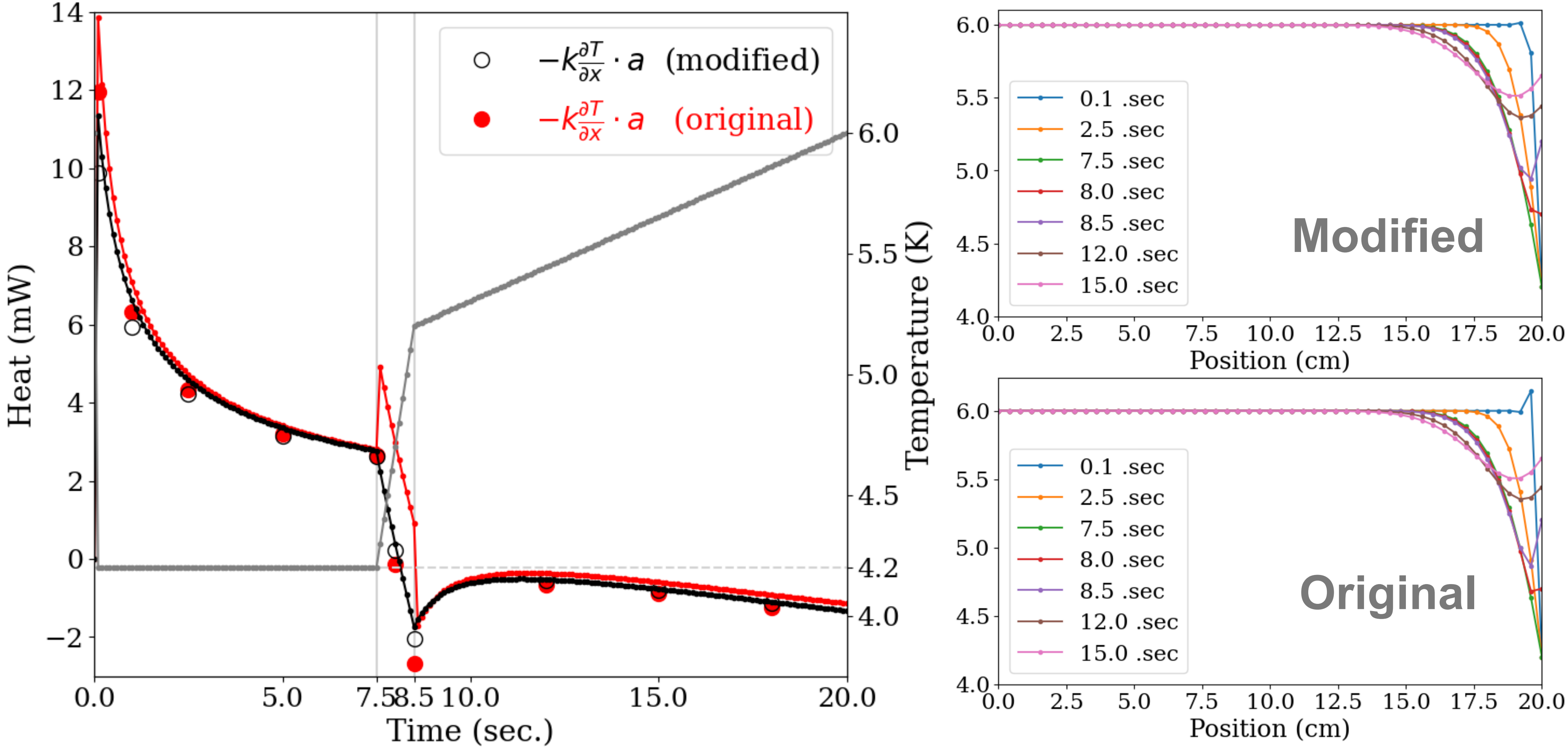
- A SUS304 wire of 0.2m (area = 1.0 cm^2)
- 50 elements (51 node)
- Initial temperature : 6 K
- Boundary temperature: Adiabatic (left end), 4.2 to 6 K (right end)







Solution scheme.. What? (2/2)



➡The original routine looks counting another amount of heat load to change the nodal temperature itself, which may bring an incorrect result <u>deviated from the net heat flow</u> out of the boundary.