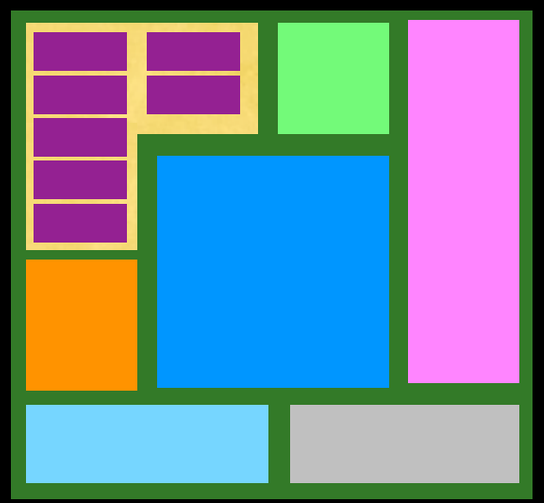
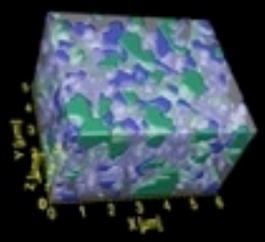


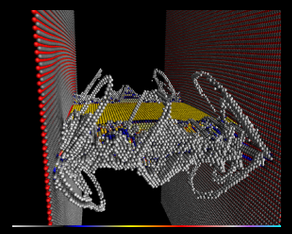
design of multiscale systems

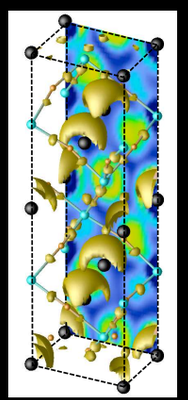
Richard LeSar & Mark Bryden

Ames Laboratory
Simulation, Modeling, and Decison Science Program

design - the materials challenge

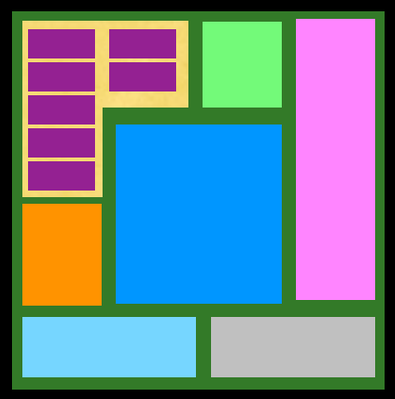






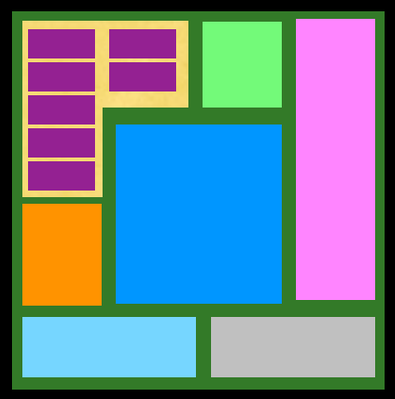
DESIGN??

??????



three big questions ...

- what is the nature of multiscale design?
- how we mathematically represent multiscale systems?
- how do we interact with multiscale systems?

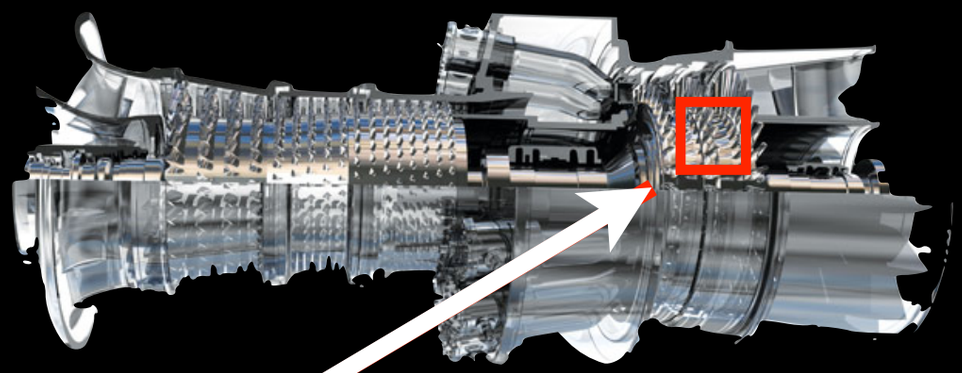


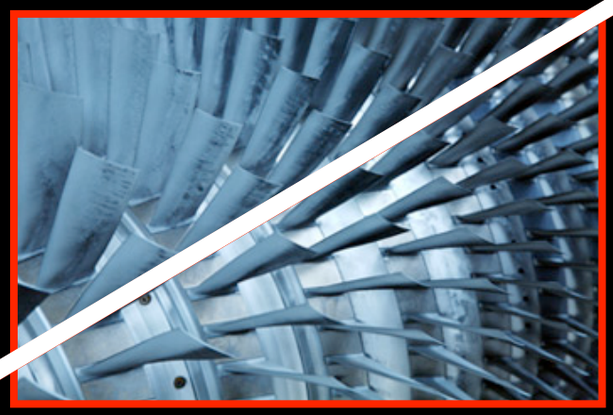
three big questions ...

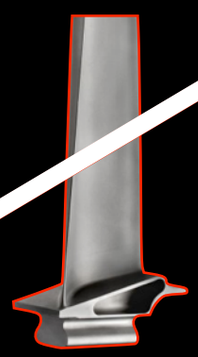
- what is the nature of multiscale design?
- how we mathematically represent multiscale systems?
- how do we interact with multiscale systems?

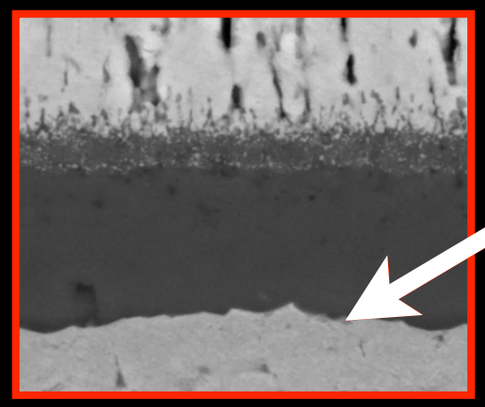
Today we cannot model the richness, fullness, or complexity of engineered, human, or natural systems.

systems of models









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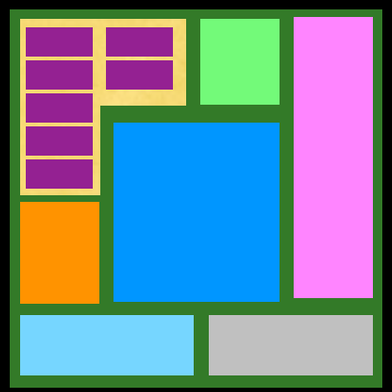
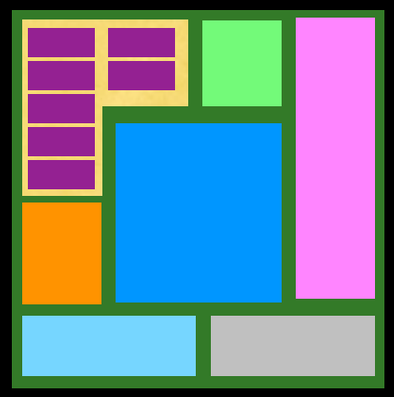
our goal

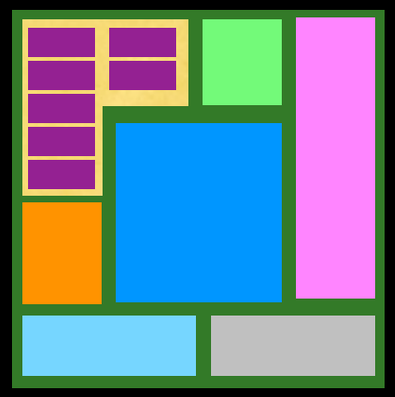


... to create a system of federated models representing the fidelity and complexity of a multiscale system



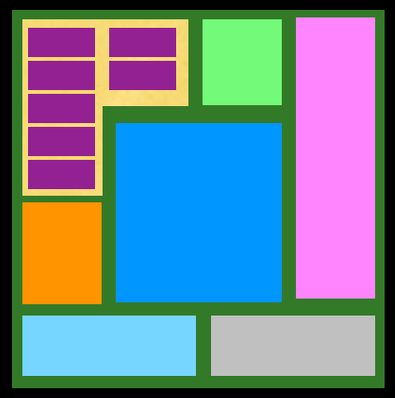
vision

- models are built at various scales by experts
- the models are used without revision
- models self identify and self assemble



self assembly

a structured organization of model systems as a consequence of local model-to-model information flow, without external direction



assumptions

- the models exist
- the data needed by each model is known and consistent with the other models in the system

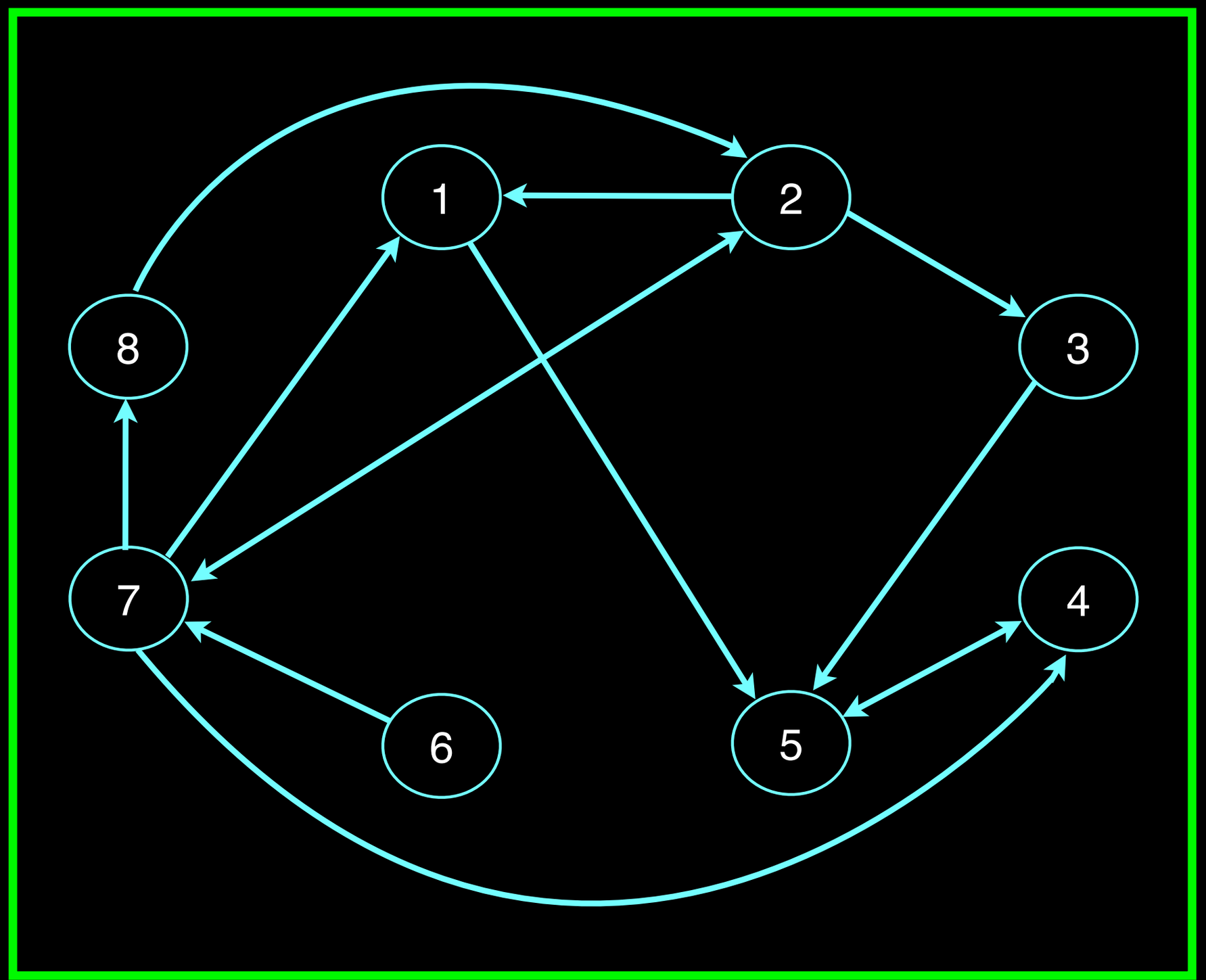
system of equations

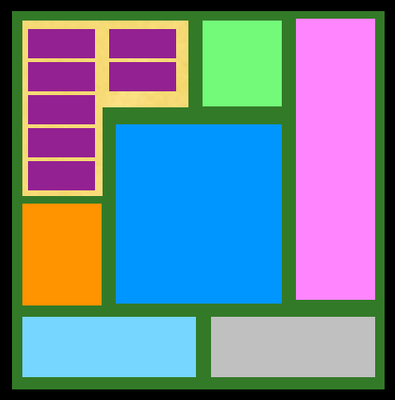
#	Equation
1	$a + b = -c$
2	$b + c = 4 - h$
3	$2b + d = 0$
4	$c + e = 10 + f$
5	$d - e + 5f = a + 3$
6	$g = 1$
7	$3b + c - g = -2h$
8	$h = c + 3$

equation	matrix

$$
\begin{array}{c}
1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8
\end{array}
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\
0 & 2 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 1 & -1 & 0 & 0 \\
-1 & 0 & 0 & 1 & -1 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 3 & 1 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & -1 & 0 & 0 & 0 & 0 & 1
\end{bmatrix}
\begin{bmatrix} a \\ b \\ c \\ d \\ e \\ f \\ g \\ h \end{bmatrix}
=
\begin{bmatrix} 0 \\ 4 \\ 6 \\ 10 \\ 3 \\ 1 \\ 0 \\ 3 \end{bmatrix}
$$

directed graph





Tarjan's algorithm

- determines the flow of information in a system of equations
- identifies strongly connected components
- used to block and schedule the solution

[1]R.E. Tarjan, "Depth-first Search and Linear Graph Algorithms," SIAM Journal of Computing 1:146-160 (1972)

system of equations

#	Equation
1	$a + b = -c$
2	$b + c = 4 - h$
3	$2b + d = 0$
4	$c + e = 10 + f$
5	$d - e + 5f = a + 3$
6	$g = 1$
7	$3b + c - g = -2h$
8	$h = c + 3$

sorted matrix

equation	matrix
1	$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 3 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 2 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & -1 & 0 & 0 \\ -1 & 0 & 0 & 1 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \\ e \\ f \\ g \\ h \end{bmatrix} = \begin{bmatrix} 0 \\ 4 \\ 0 \\ 6 \\ 10 \\ 3 \\ 1 \\ 3 \end{bmatrix}$

connection matrix

equation	connection matrix
1	$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \\ e \\ f \\ g \\ h \end{bmatrix}$
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blocked connection matrix

equation	connection matrix
6	$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} g \\ c \\ b \\ h \\ a \\ d \\ e \\ f \end{bmatrix}$
7	
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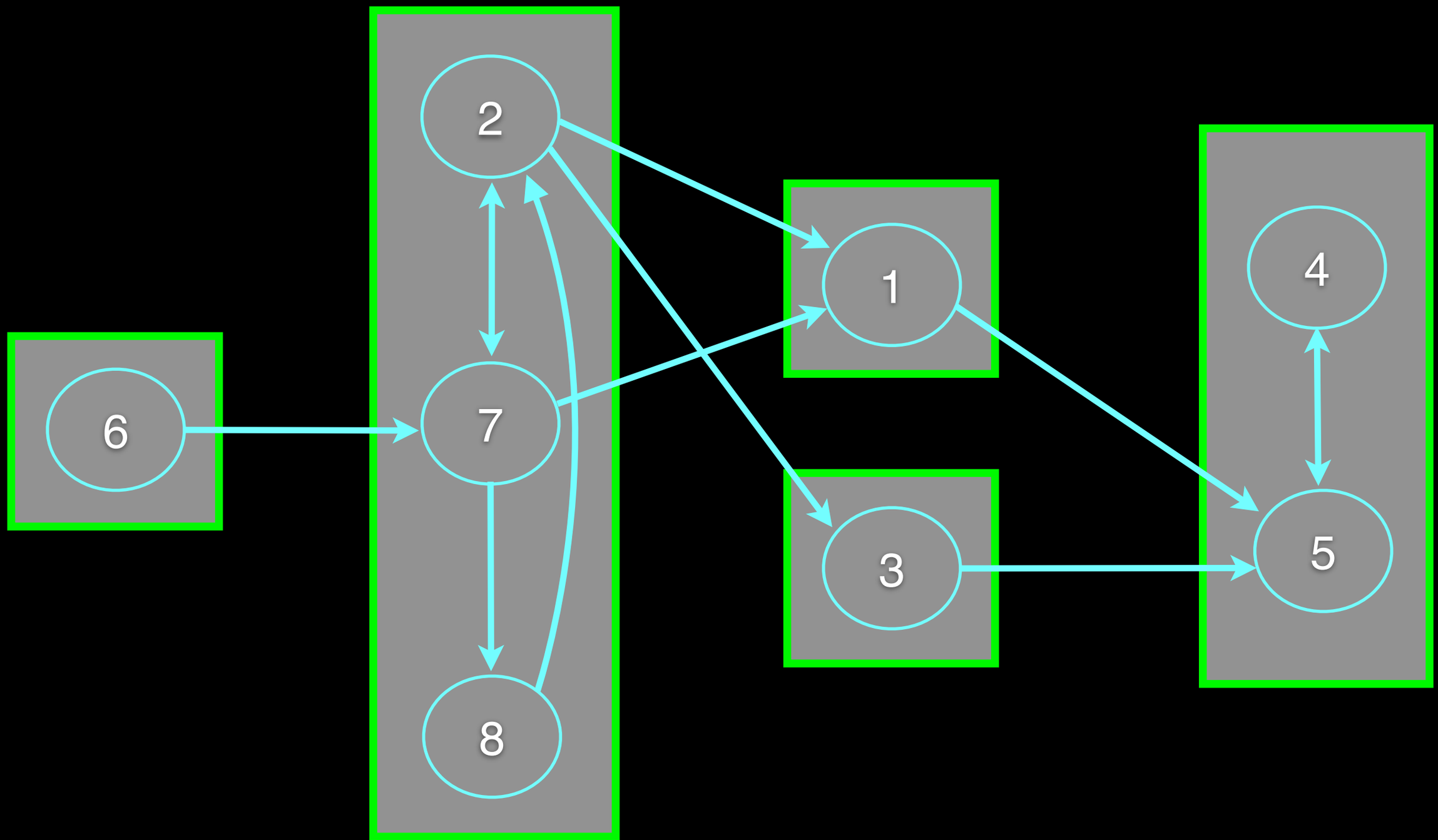
blocked connection matrix

equation	connection matrix								
6	1	0	0	0	0	0	0	0	g
7	1	1	1	0	0	0	0	0	c
2	0	1	1	1	0	0	0	0	b
8	0	1	0	1	0	0	0	0	h
1	0	1	1	0	1	0	0	0	a
3	0	0	1	0	0	1	0	0	d
4	0	1	0	0	0	0	1	1	e
5	0	0	0	0	1	1	1	1	f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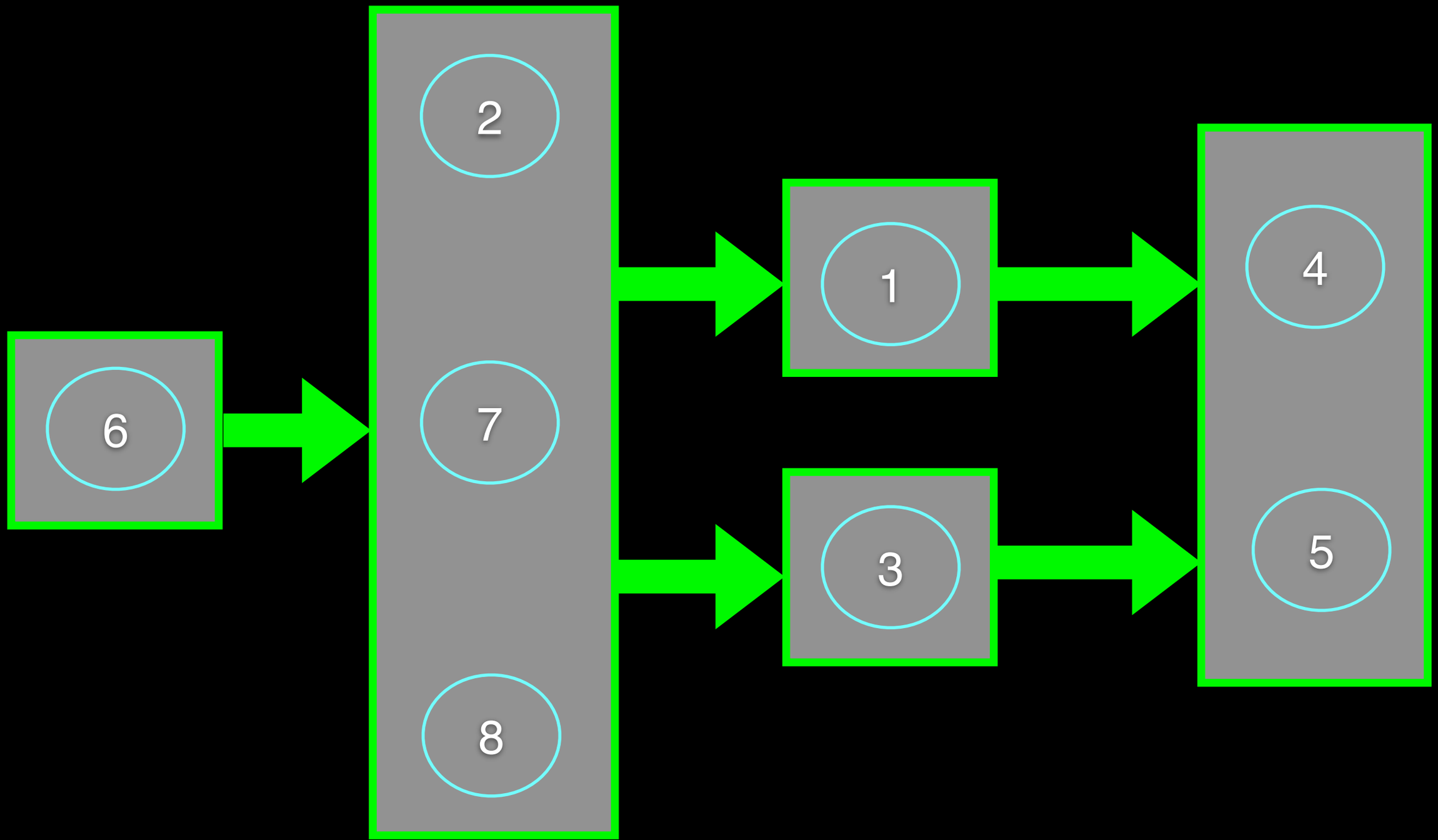
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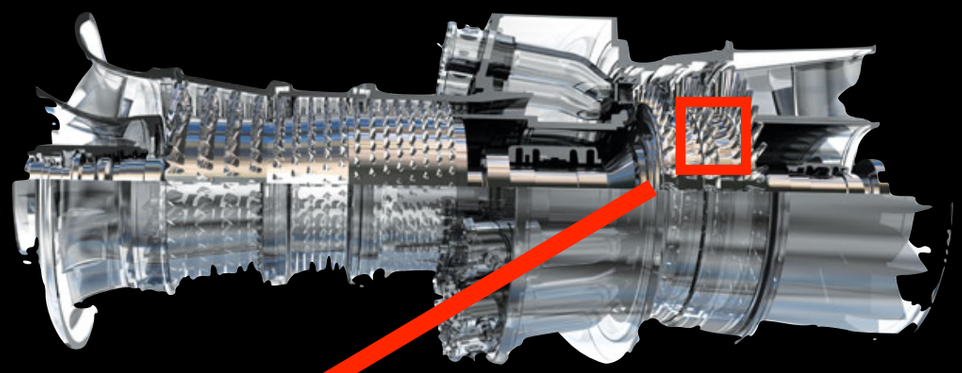
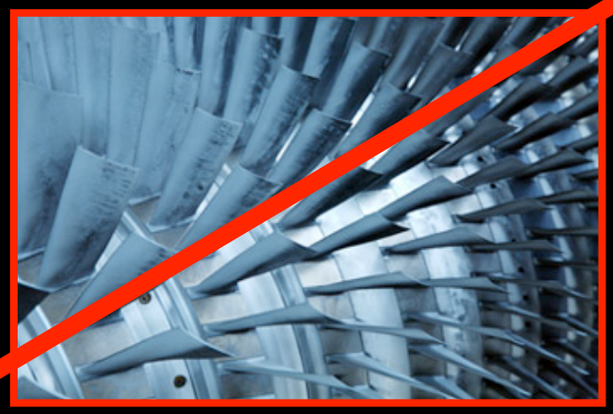
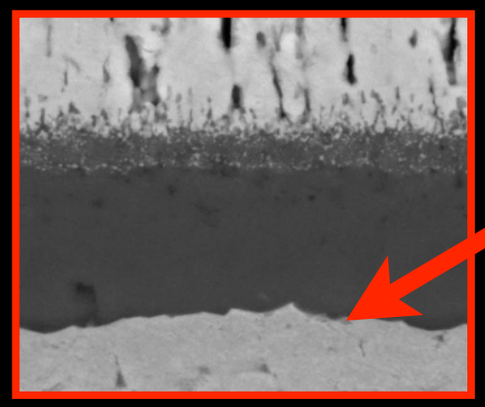
systems of models







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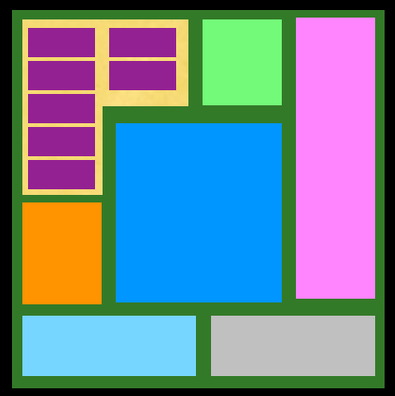
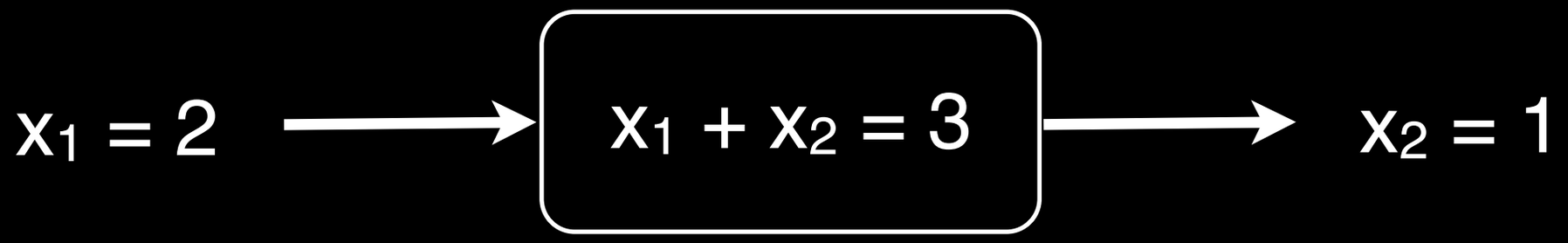
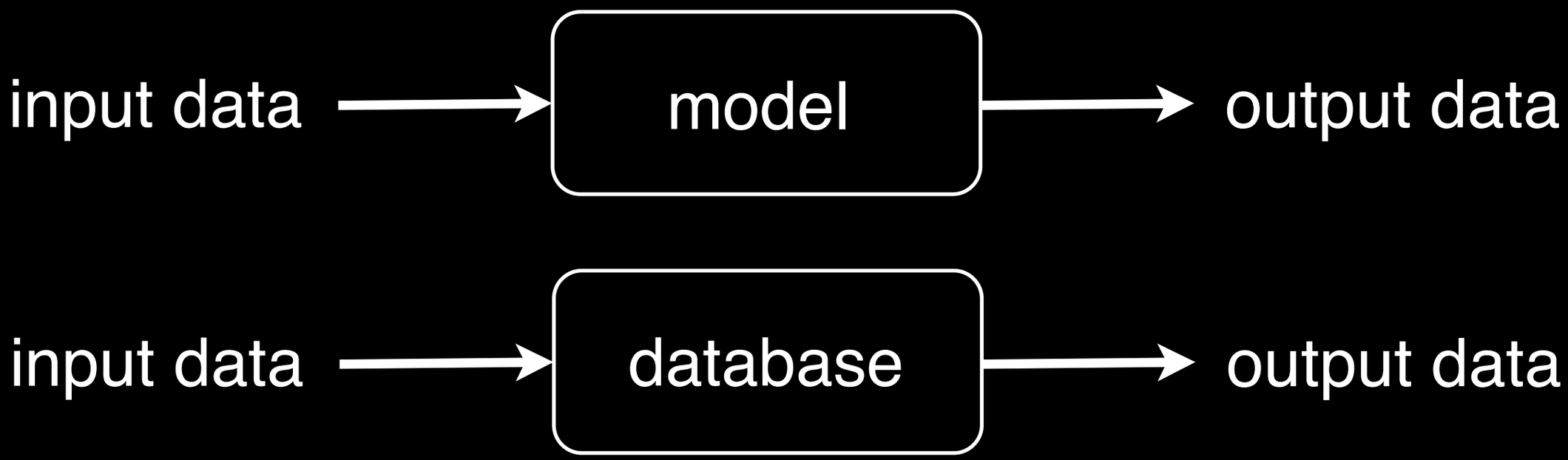
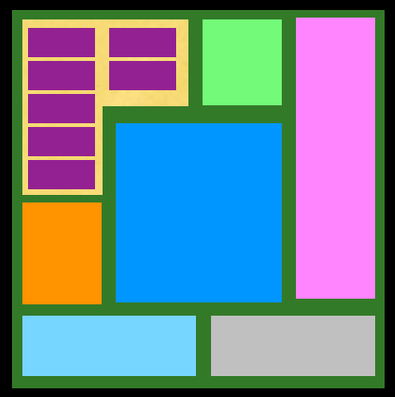


it’s all just information

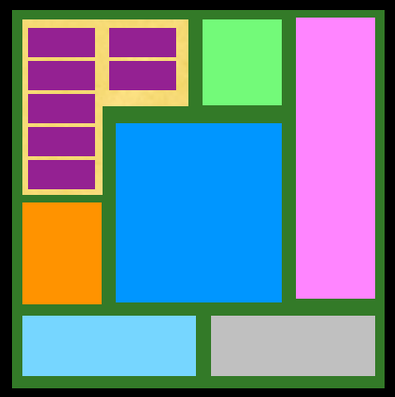






information entities

- models
- simulations
- databases
- sensors
- ...

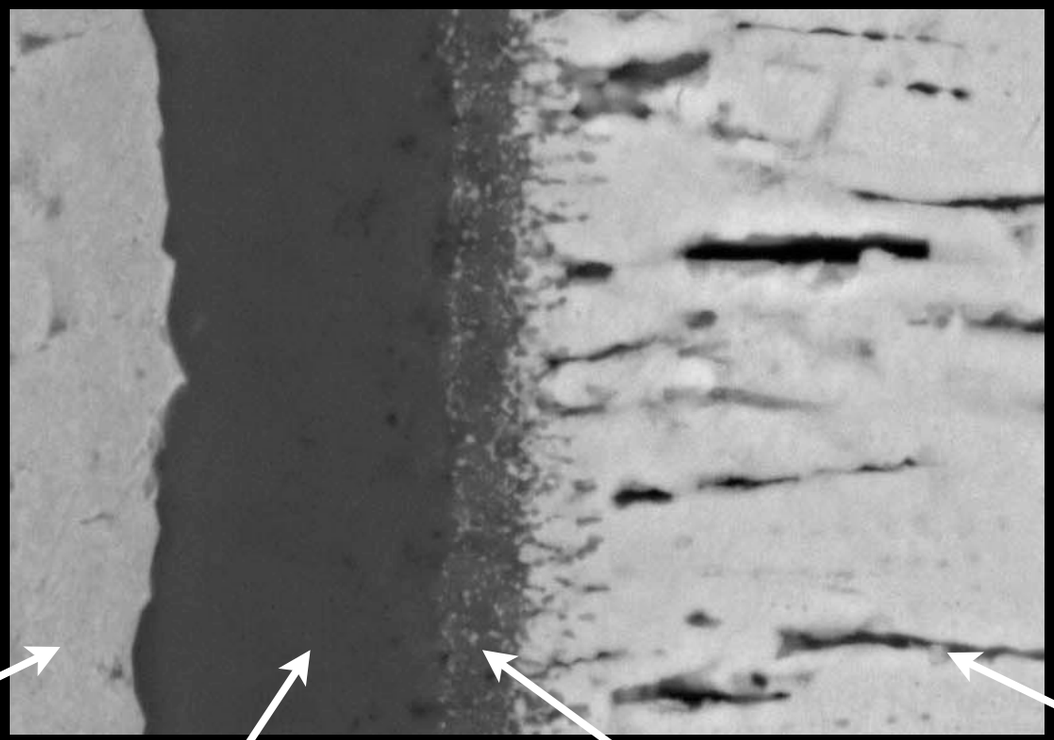


extended Tarjan's algorithm

- identifies information flow in a complex computational system
- identifies groupings
- organizes and schedules order of operation

turbine blade

internal
cooling air



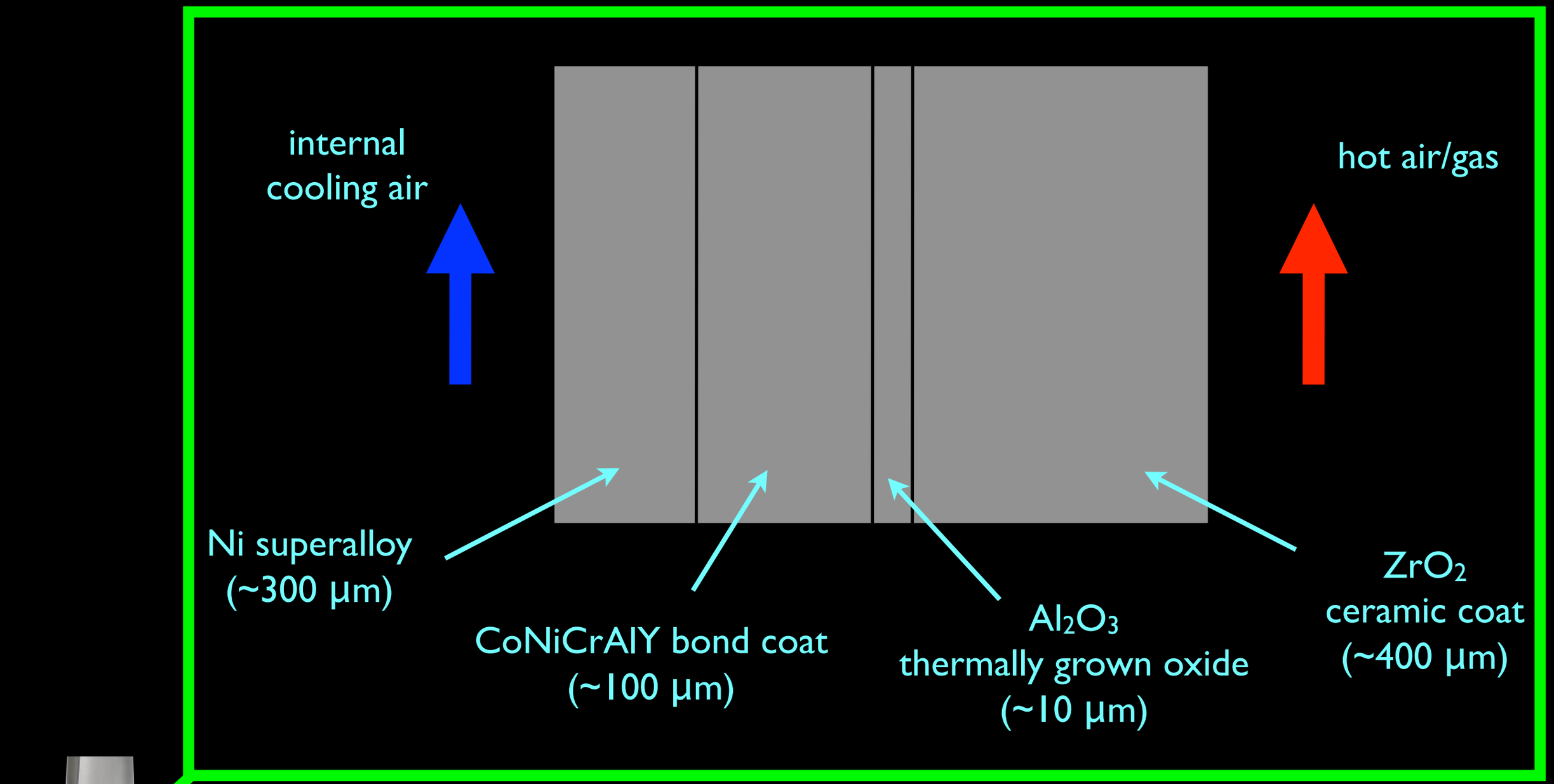
hot air/gas

Ni superalloy
(~300 μm)

CoNiCrAlY bond coat
(~100 μm)

Al_2O_3
thermally grown oxide
(~10 μm)

ZrO_2
ceramic coat
(~400 μm)


internal
cooling air
hot air/gas
Ni superalloy
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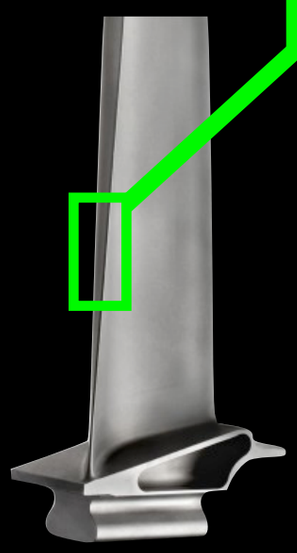
ceramic coat
(~400 μm)



1 Convective heat transfer equation for (cooling air)

2 Substrate properties database

3 1D FVM solver for thermal diffusion in the substrate layer

4 1D FVM solver for thermal stress in the substrate layer

5 Bond coat material properties database

6 1D FVM solver for thermal diffusion in the bond coat

7 1D FVM solver for thermal stress in the bond coat

8 TGO layer material properties database

9 1D FVM solver for thermal diffusion in TGO layer

10 1D FVM solver for thermal stress in the bond coat

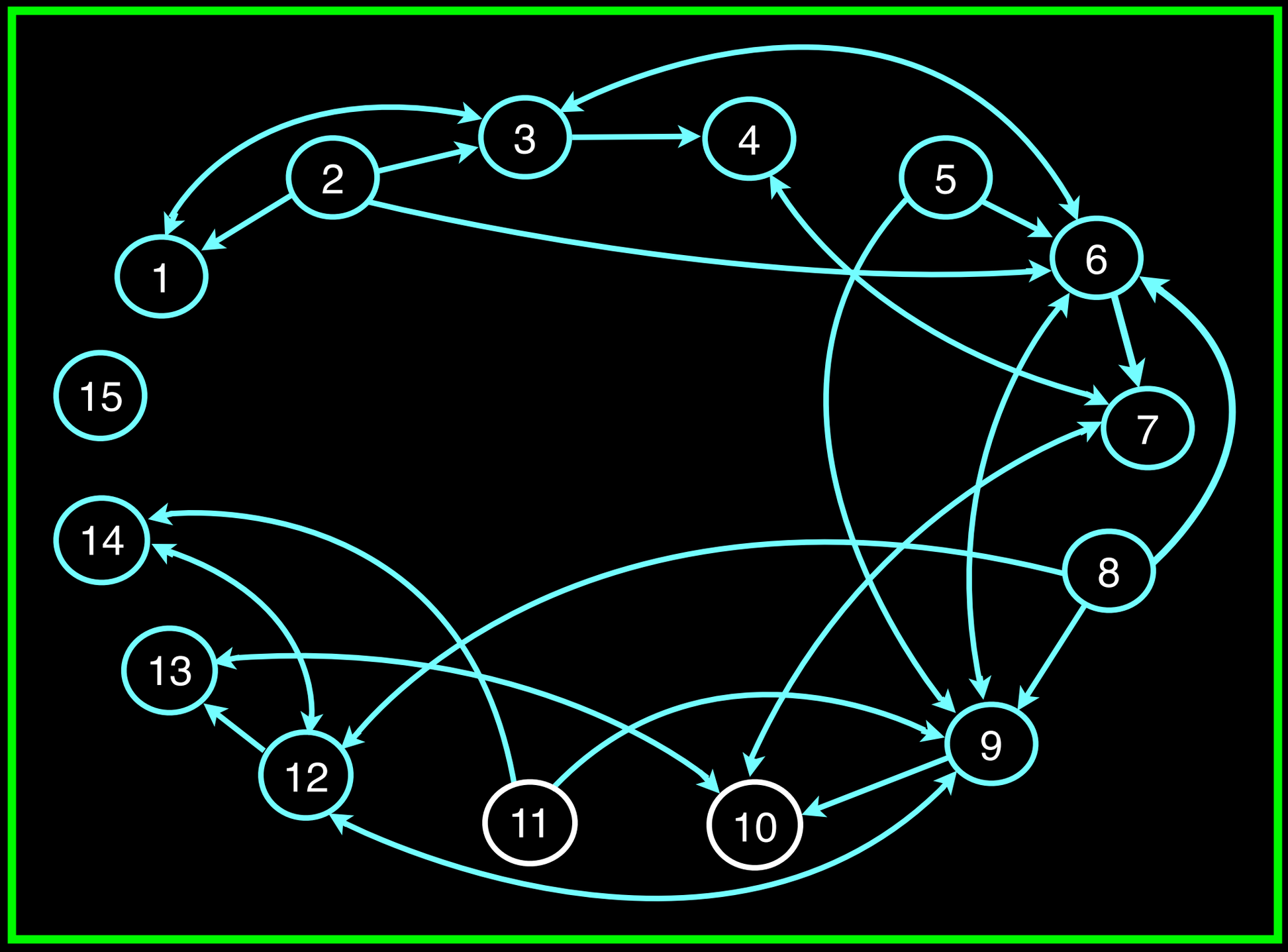
11 Ceramic topcoat material properties database

12 1D FVM solver for thermal diffusion in the ceramic topcoat

13 1D FVM solver for thermal stress in the ceramic topcoat

14 Convective heat transfer equation (hot air)

15 TBC material cost model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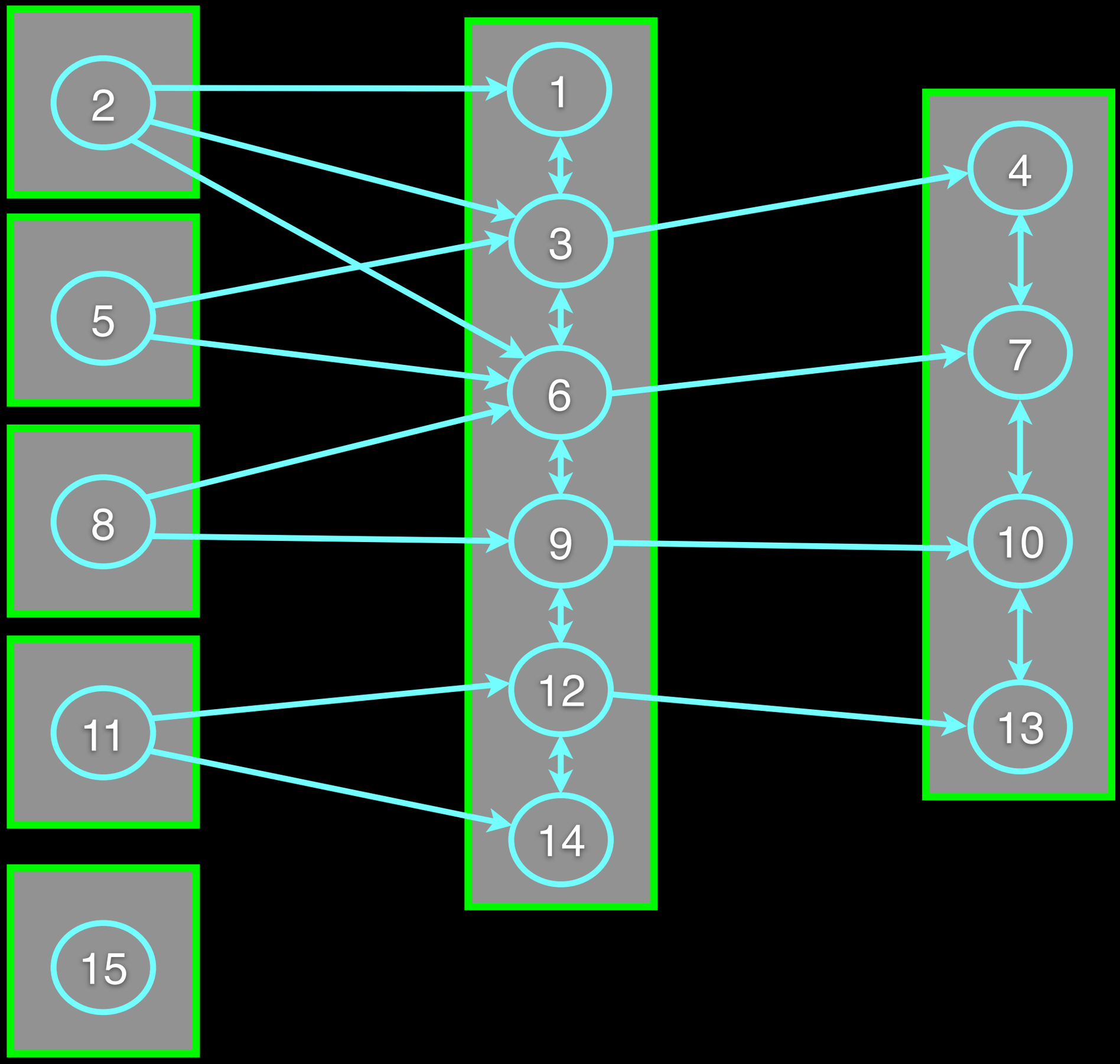
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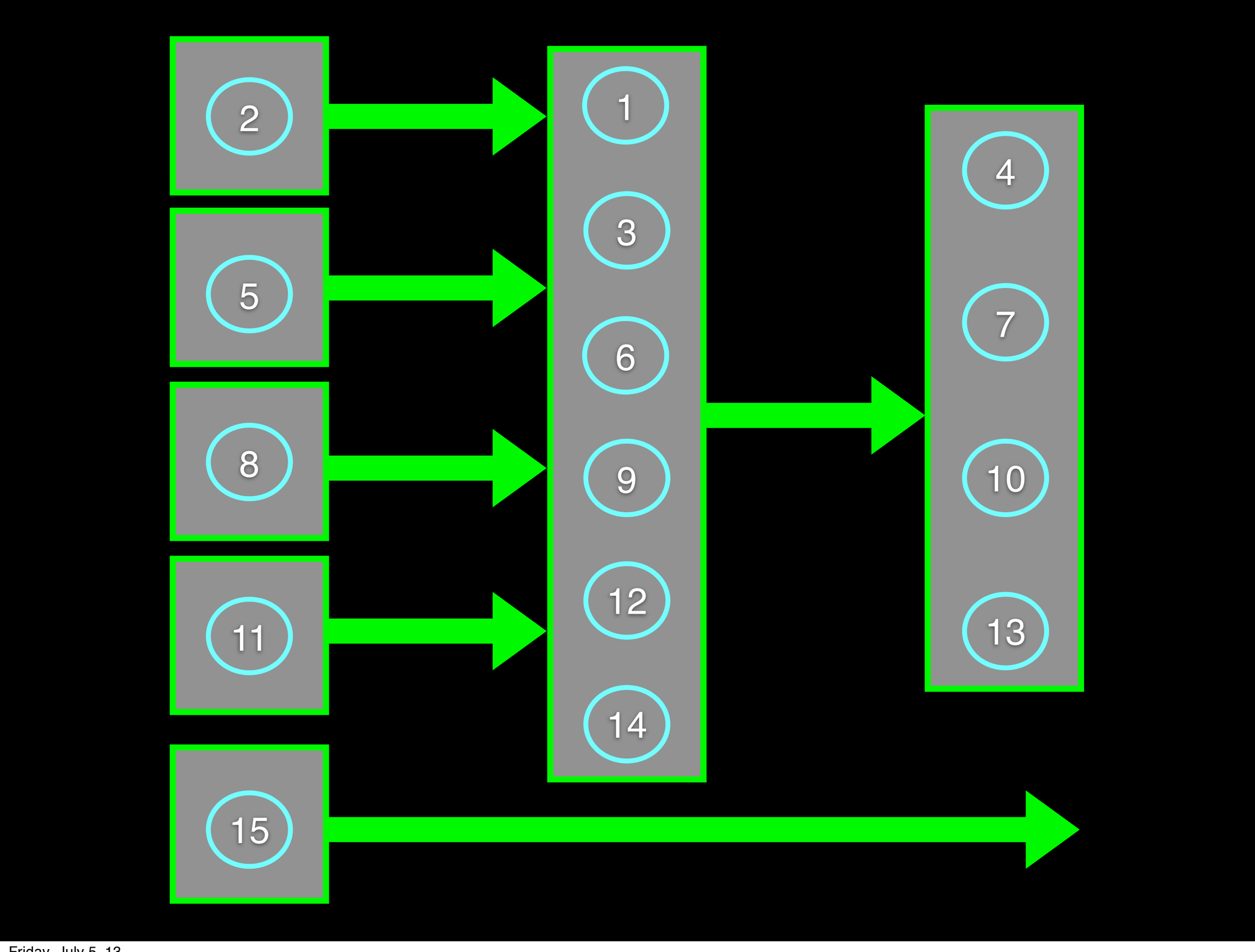
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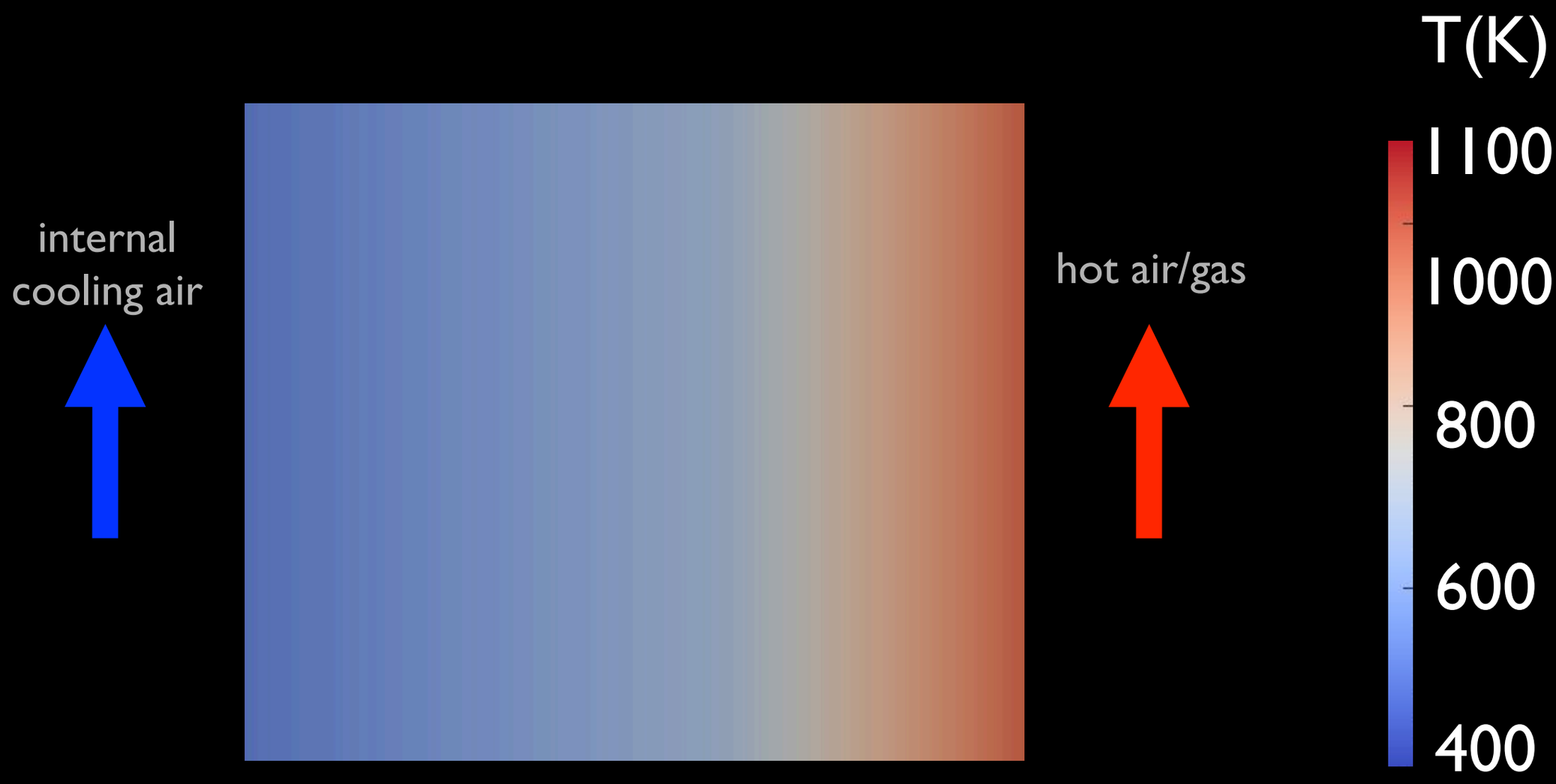
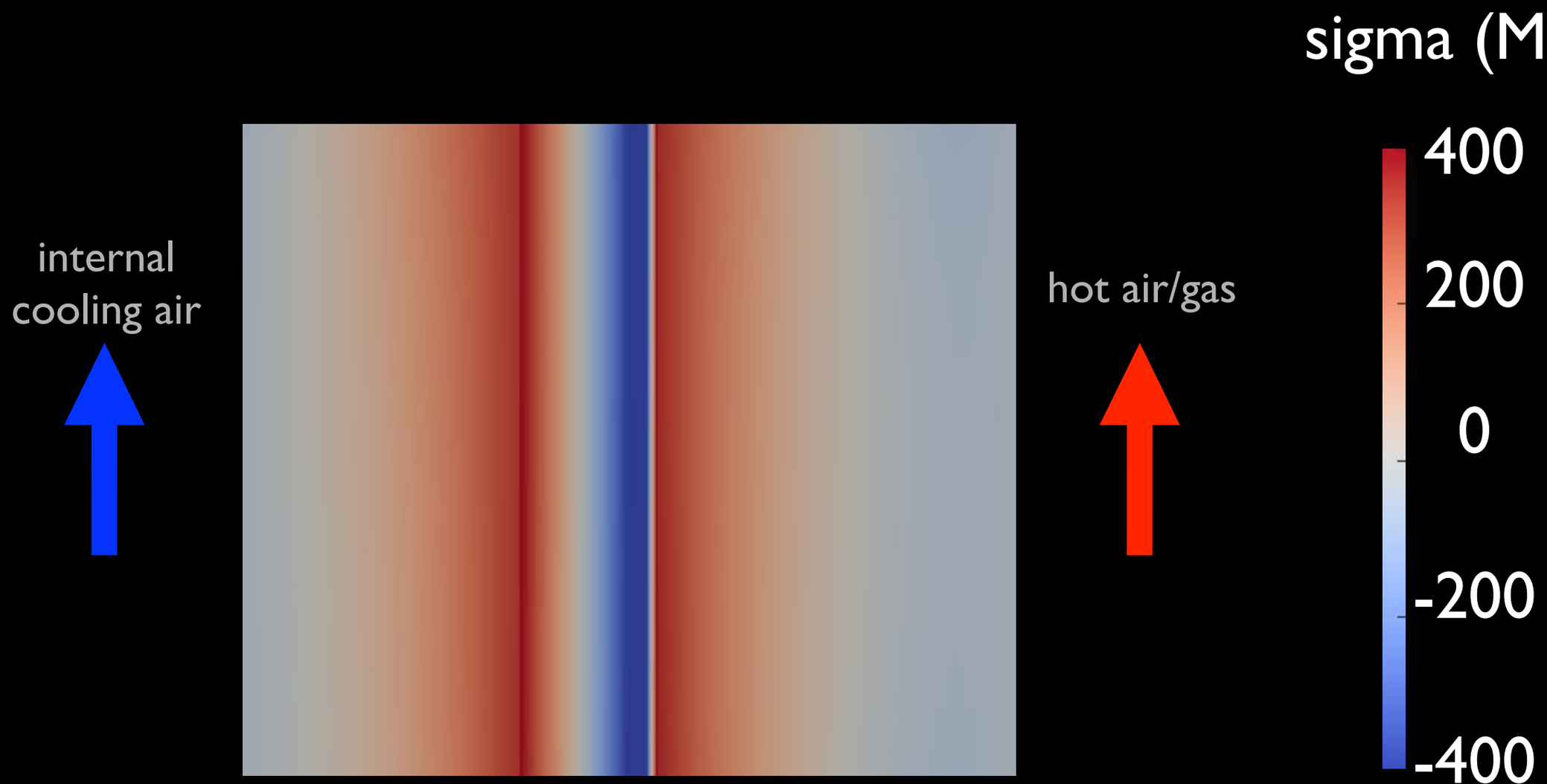
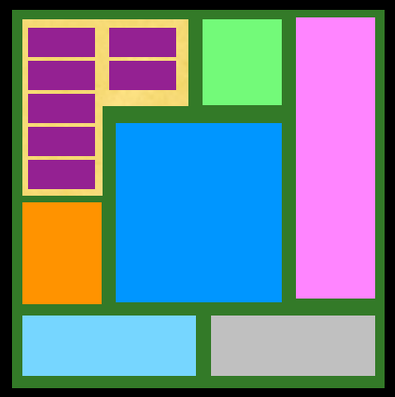
temperature distribution



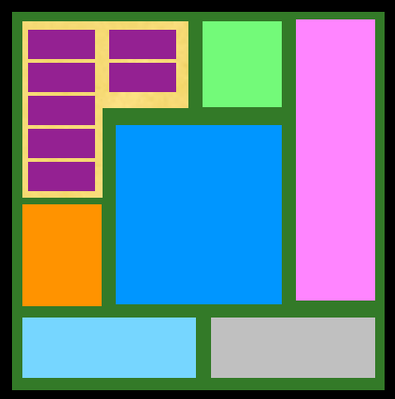
thermal shear stress





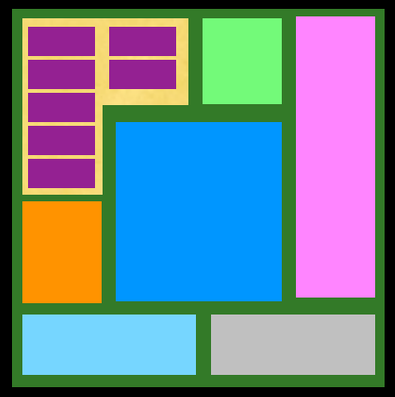
conclusions

- Tarjan’s algorithm can be extended to identify the information flow in complex computational systems
- extensible to multiscale modeling of gas turbines, steam turbines, boiler tubes, sensors ...



future work

- self identification
- resource allocation
- reduced-order models
- integration into multiscale design process



questions?