# COMPUTATIONAL THERMAL ANALYSIS

## PRESENTATION MEDIA SAMPLE

Selection Featured in Lecture 5a



Engineering Short Course

www.TITANAlgorithms.com/courses.html

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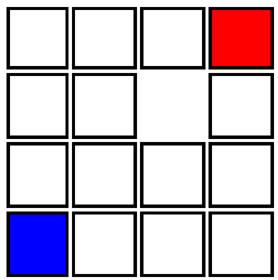
# ***Time Discretization***

# TIME DISCRETIZATION
## *Pictorial*

- **Time Discretization**: *a process of converting the continuous time derivative into a discrete time derivative*



$$(\rho \cdot C_P \cdot \delta V)_i \cdot I \cdot \frac{d}{dt} T = G \cdot T + S$$

time discretization

$$(\rho \cdot C_P \cdot \delta V)_i \cdot I \cdot \frac{T^{<n>} - T^{<n-1>}}{\Delta t} = G \cdot T^{<q>} + S$$

time level n, n-1 and to be defined level, q

solve discrete space-time equation numerically
essence of computational heat transfer

# TIME DISCRETIZATION

## *Specifying the Time Level q*

- Convert the vectorized conservation equation to discrete time derivative
  - ➢ define discrete time levels are denoted using superscripts *(n)*
    - - $\boldsymbol{T}^{(q)}$ is the temperature vector
    - - registered at a discrete time $q\ \Delta t \quad example\ 1\Delta t,\ 2\Delta t,\ \ldots$
  - ➢ convert the time derivative by reaching backwards in time by *1Δt*

**➡ *What should we select q to be?***

- **Foward Differencing**: *for this exercise we will set q to be n (q = n) current present time (reason explained below)*

$$\frac{d}{dt}\boldsymbol{T} - \boldsymbol{A}\ \boldsymbol{T} = \boldsymbol{f} \quad \Longrightarrow \quad \frac{\boldsymbol{T}^{(n)} - \boldsymbol{T}^{(n-1)}}{\Delta t} - \boldsymbol{A}\ \boldsymbol{T}^{(n)} = \boldsymbol{f}$$

$$where \quad \boldsymbol{A} = \boldsymbol{C}^{-1}\ \boldsymbol{G}$$

$$\boldsymbol{f} = \boldsymbol{C}^{-1}\ \dot{\boldsymbol{S}}$$

*forward time differencing*

# TIME DISCRETIZATION

## *Define the Time Step Δt*

- We can define the discrete value of $\Delta t$ to be any value we wish:
  - define $\Delta t \rightarrow \infty$ that is, evaluate the above equation by setting the time spacing to infinity
  - this has the effect of moving from the initial vector of temperatures to the final vector out at infinite time in one big time step
  - in other words $\boldsymbol{T}^{(n\rightarrow\infty)} \equiv \boldsymbol{T}_{SteadyState}$

- Set $\Delta t \rightarrow \infty$ and simplify the discrete equation:

$$\lim_{\Delta t\rightarrow\infty}\left(\frac{\boldsymbol{T}^{(n)} - \boldsymbol{T}^{(n-1)}}{\Delta t} - \boldsymbol{A}\,\boldsymbol{T}^{(n)}\right) = \boldsymbol{f} \quad\Longrightarrow\quad \boldsymbol{A}\,\boldsymbol{T}^{(n\rightarrow\infty)} + \boldsymbol{f} = 0$$

➡ ***Note that we applied a transient solution to derive the steady state equation using a single infinitely large time step***

# TIME DISCRETIZATION

## *Evaluating Equation at Infinite Δt*

- Substituting the equations for the ***A*** and ***f*** matrices and rearrange:
  - capacitance matrix cancels out as expected
  - same equation derived in the direct solution method

$$C^{-1} G\ T^{(n \to \infty)} + C^{-1} \dot{S} = 0$$

$$G\ T^{(n \to \infty)} + \dot{S} = 0$$

- Note that we cannot invert ***G*** directly as we could in the direct solution method:
  - we are now reverting to full numerical methods
  - ***G*** is a very long stacked vector (elements = # of CVs)
    - matrix operations no longer suitable as we described above
    - must invert numerically

➥ ***Note that the essence of all CTA numerical solutions is a gradual inversion of the conductance matrix - gradual in the sense that a single direct inversion is no longer possible***

# STEADY STATE SOLUTIONS
## *Residual Form*

- **Residual Form**: *a variation of the basic vectorized energy equation where the form of the equation is rewritten to accommodate an energy imbalance*

$$\Rightarrow \quad \varphi = G\,\tilde{T} + \dot{S}$$

- **Solution residual φ**: *a vector which represents the energy imbalance in each of the linear equations*
  - $\tilde{T}$ is a provisional solution en route to the final steady state solution $T^{(\infty)}$
  - **Objective**: to drive $\varphi \rightarrow 0$
  - residual vector will have finite numbers
    - units of energy rate (Watts)
    - direct measure of convergence

➡ ***As will be shown, the residual form approach can be applied to nonlinear systems of equations as well***

# SOLVING THE RESIDUAL FORM
## *Generalized Newton's Method*

- Apply a ***Generalized Newton's*** (GN) Method to solve the residual equation

$$\varphi(\tilde{T}) = G\,\tilde{T} + \dot{S} = 0$$

- **GN Method**: *solves the $i^{th}$ equation for $\varphi_i$ for the $i^{th}$ unknown value of* $\tilde{T}_i$
  - the generalized Newton's method works on a partial of the residual with respect to target unknown
  - energy residual used to generate small adjustments in the temperature vector
  - GN form is applicable when the residual equation is nonlinear

$$\tilde{T}_i^{(m\ iteration)} = \tilde{T}_i^{(m-1\ iteration)} - \omega\,\frac{\varphi_i(\tilde{T}_i)}{\dfrac{\partial\varphi_i(\tilde{T}_i)}{\partial\tilde{T}_i}}$$

# SOLVING THE RESIDUAL FORM
## *Generalized Newton's Method - Notes*

$$\tilde{T}_i^{(m\ iteration)} = \tilde{T}_i^{(m-1\ iteration)} - \omega \frac{\varphi_i(\tilde{T}_i)}{\frac{\partial \varphi_i(\tilde{T}_i)}{\partial \tilde{T}_i}}$$

- Two basic components
  - present iteration state
  - relaxation term
- Term ω is defined as the ***successive over-relaxation*** factor (SOR)
  - ω can be greater or less than 1
  - ω = 1 then method reverts to ***Gauss Seidel Iteration***
- Iteration counter superscript (m):
  - similar to the discrete time counter (n)
  - the residual equations will progress through what appears to be transients

# SOLVING THE RESIDUAL FORM
## *Coldplate Example*

- Apply the restructured form of the equations and generate the residual vector

$$\varphi(\tilde{T}) = G\,\tilde{T} + \dot{S}$$
$$= 0$$

$$\phi = \begin{bmatrix} -6 & 2 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & -6 & 2 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & -4 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -6 & 2 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 2 & -8 & 2 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 2 & -6 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 2 & -6 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & -6 & 2 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 2 & -6 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & -4 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & -4 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 2 & -6 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & -4 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 2 & -4 \end{bmatrix} \cdot \begin{bmatrix} T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \\ T_7 \\ T_8 \\ T_9 \\ T_{10} \\ T_{11} \\ T_{12} \\ T_{13} \\ T_{14} \\ T_{15} \end{bmatrix} + \begin{bmatrix} 2\cdot T_B \\ 0 \\ 0 \\ 2\cdot T_B \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 100 \end{bmatrix}$$

$$\begin{bmatrix} \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \\ \phi_6 \\ \phi_7 \\ \phi_8 \\ \phi_9 \\ \phi_{10} \\ \phi_{11} \\ \phi_{12} \\ \phi_{13} \\ \phi_{14} \\ \phi_{15} \end{bmatrix} = \begin{bmatrix} -6\cdot T_2 + 2\cdot T_3 + 2\cdot T_6 + 2\cdot T_B \\ 2\cdot T_2 - 6\cdot T_3 + 2\cdot T_4 + 2\cdot T_7 \\ 2\cdot T_3 - 4\cdot T_4 + 2\cdot T_8 \\ -6\cdot T_5 + 2\cdot T_6 + 2\cdot T_9 + 2\cdot T_B \\ 2\cdot T_2 + 2\cdot T_5 - 8\cdot T_6 + 2\cdot T_7 + 2\cdot T_{10} \\ 2\cdot T_3 + 2\cdot T_6 - 6\cdot T_7 + 2\cdot T_8 \\ 2\cdot T_4 + 2\cdot T_7 - 6\cdot T_8 + 2\cdot T_{11} \\ 2\cdot T_5 - 6\cdot T_9 + 2\cdot T_{10} + 2\cdot T_{12} \\ 2\cdot T_6 + 2\cdot T_9 - 6\cdot T_{10} + 2\cdot T_{13} \\ 2\cdot T_8 - 4\cdot T_{11} + 2\cdot T_{15} \\ 2\cdot T_9 - 4\cdot T_{12} + 2\cdot T_{13} \\ 2\cdot T_{10} + 2\cdot T_{12} - 6\cdot T_{13} + 2\cdot T_{14} \\ 2\cdot T_{13} - 4\cdot T_{14} + 2\cdot T_{15} \\ 2\cdot T_{11} + 2\cdot T_{14} - 4\cdot T_{15} + 100 \end{bmatrix}$$

- Apply residual vector to GN method to derive the temperature iteration equation
  - ➢ simplify by setting $\omega = 1$
  - ➢ note partial derivatives are just constants (the diagonals of ***G***)

General Residual Equation i: $T_i^{<n>} = T_i^{<n-1>} - \omega \cdot \dfrac{\phi_i(\mathbf{T})}{\dfrac{\partial \phi_i(\mathbf{T})}{\partial T_i}}$

General Residual Equation 2:

$$T_2^{<n>} = T_2^{<n-1>} - \omega \cdot \frac{\left(2 \cdot T_B - 6 \cdot T_2 + 2 \cdot T_3 + 2 \cdot T_6\right)}{\frac{\partial\left(2 \cdot T_B - 6 \cdot T_2 + 2 \cdot T_3 + 2 \cdot T_6\right)}{\partial T_2}}$$

$$T_2^{<n>} = T_2^{<n-1>} + \frac{\omega}{6} \cdot \left(2 \cdot T_B - 6 \cdot T_2^{<n-1>} + 2 \cdot T_3 + 2 \cdot T_6\right)$$

$$T_2^{<n>} = (1 - \omega) \cdot T_2^{<n-1>} + \frac{\omega}{6} \cdot \left(2 \cdot T_B + 2 \cdot T_3 + 2 \cdot T_6\right)$$

for ω=1 we get the expression: $T_2^{<n>} = \frac{1}{6} \cdot \left(2 \cdot T_B + 2 \cdot T_3 + 2 \cdot T_6\right)$

General Residual Equation 3:

$$T_3^{<n>} = T_3^{<n-1>} - \omega \cdot \frac{\left(2 \cdot T_2 - 6 \cdot T_3 + 2 \cdot T_4 + 2 \cdot T_7\right)}{\frac{\partial\left(2 \cdot T_2 - 6 \cdot T_3 + 2 \cdot T_4 + 2 \cdot T_7\right)}{\partial T_3}}$$

$$T_3^{<n>} = (1 - \omega) \cdot T_3^{<n-1>} + \frac{\omega}{6} \cdot \left(2 \cdot T_2 + 2 \cdot T_4 + 2 \cdot T_7\right)$$

for ω=1 we get the expression: $T_3^{<n>} = \frac{1}{6} \cdot \left(2 \cdot T_2 + 2 \cdot T_4 + 2 \cdot T_7\right)$

# SOLVING THE GN EQUATIONS

## *Coldplate Discretization Example*

- Start with an arbitrary selection of the initial temperatures
  - ➢ set all values of T=0
  - ➢ Boundary CV-1
    - define $T_B = 20\ °C$
    - residual automatically satisfied $\varphi_1 \equiv 0$

- **Iterate Solution**: *use the most recent values of the provisional temperature solution*
  - ➢ **Example**: *when iterating the 4th equation* $\varphi_4$ *apply the most recently determined values of* $\tilde{T}_1$ , $\tilde{T}_2$ , $\tilde{T}_3$ *since these should be known*
  - ➢ continue the iteration until the ***stopping criterion*** is meet (discussed below)

**ANIMATION DISPLAY**

Evolution of Steady State Solution - SOR = 1

**ANIMATION DISPLAY**

Evolution of Steady State Solution - SOR = 1.95

**ANIMATION DISPLAY**

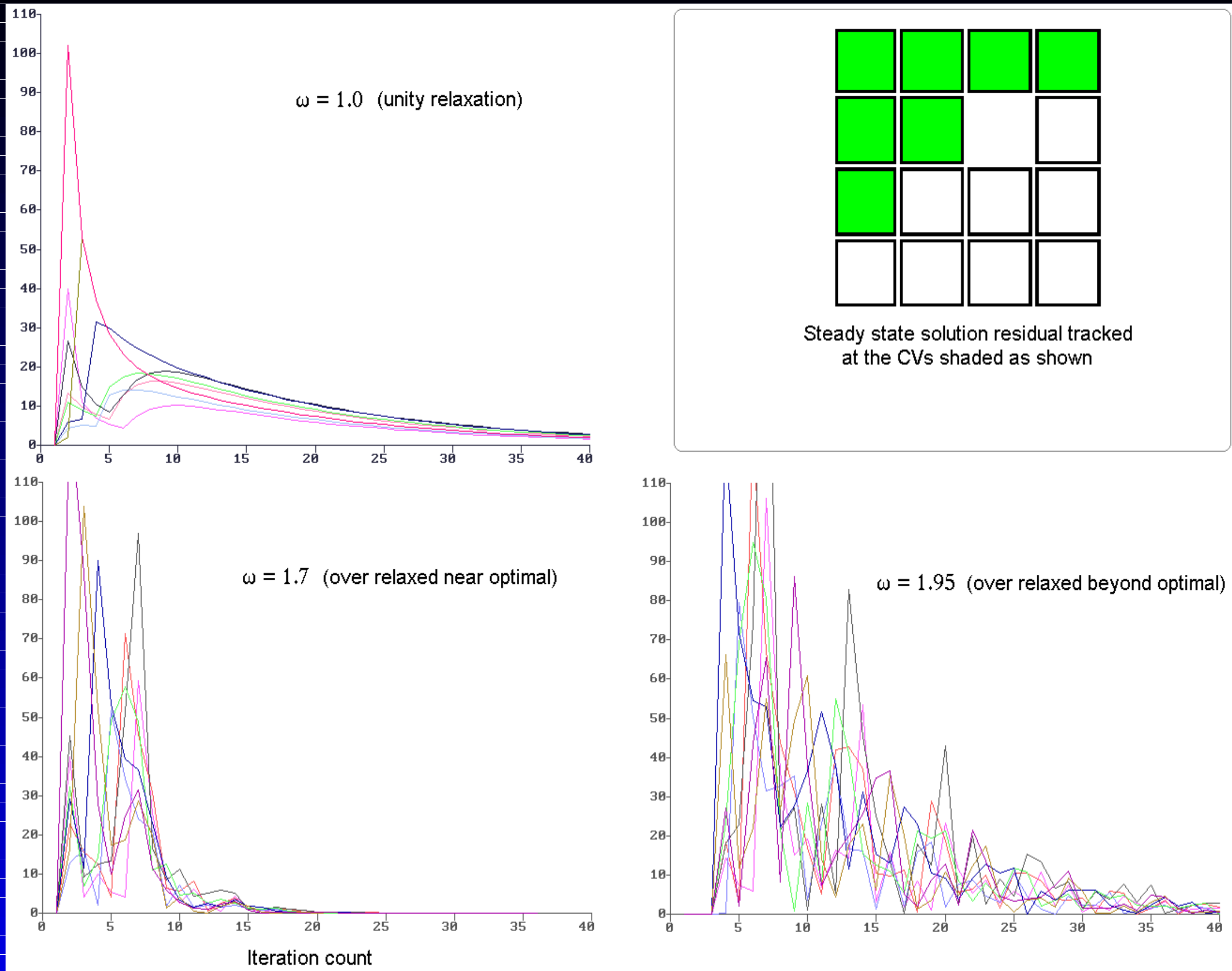
Evolution of Steady State Solution - SOR = 1.7

# MAPPING SOLUTION RESIDUALS
## *Steady State*

- Compare the local and ***vector-norm*** of the residuals at each iteration pass of all 14 equations:

$$\text{vector norm of the residuals} \quad |\boldsymbol{\varphi}| = \frac{1}{N}\sqrt{\sum_{i=1}^{N} \varphi_i^2}$$

- **Residual elimination**:
  - ➢ residuals are driven to zero with successive iteration sweeps through the set of 14 equations
  - ➢ appears to be an optimal ω which minimizes the number of iterations




*Solution residuals with each iteration of the GN equations showing effect of relaxation factor*

Note that we are observing the solution residual and not the temperature. The residual is a measure of numerical energy imbalance in the steady state solution.

**ANIMATION DISPLAY**

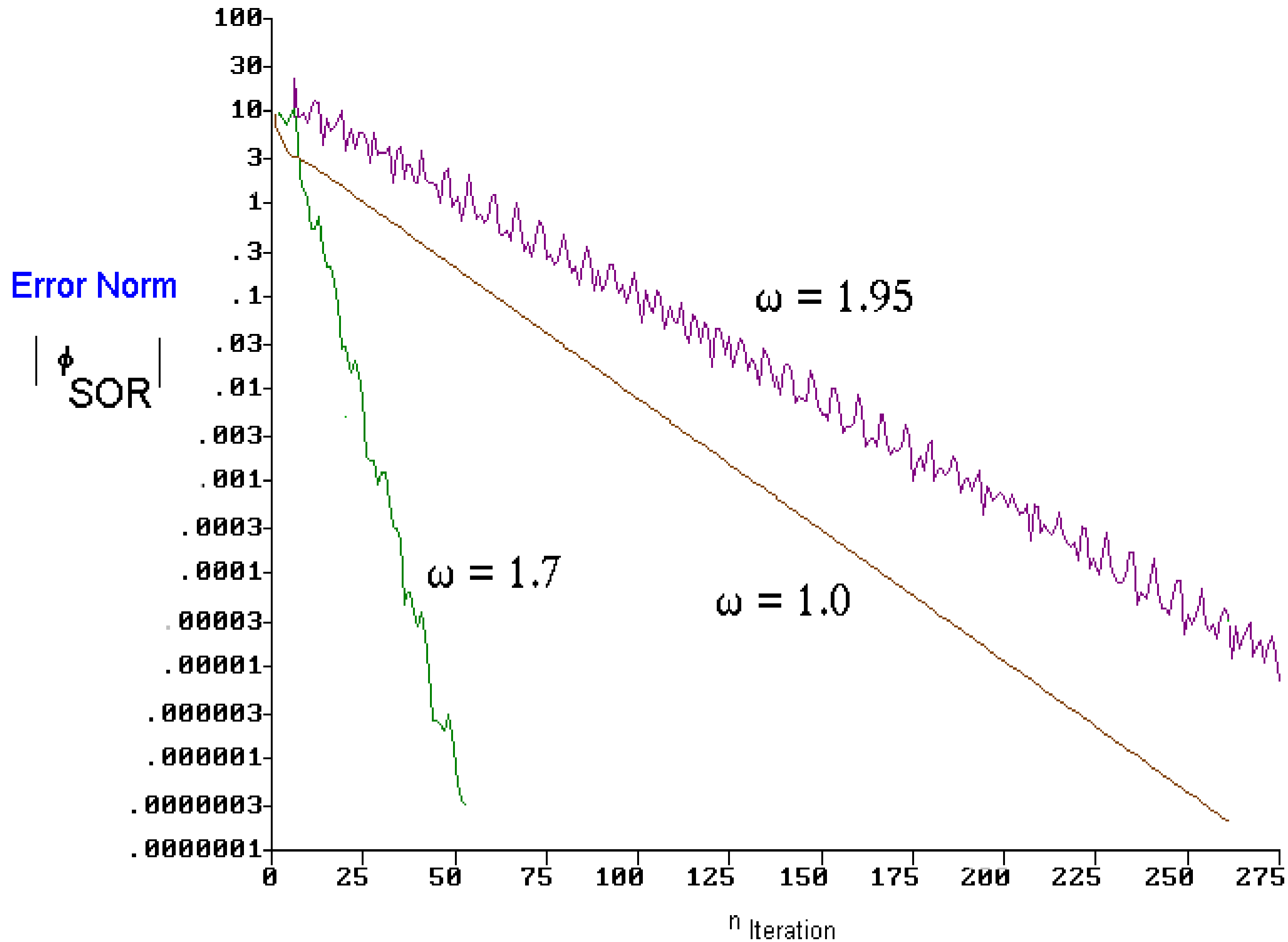
Evolution of Solution Residuals

Note the propagation of the solution residual as it moves through the solution domain. Residuals diffuse in a manner similar to energy.

Note how the residual appears to rebound off the wall in this corner

**ANIMATION DISPLAY**

Evolution of Solution Residuals




Effect of relaxation factor on steady state residual norms using relaxation solution method

*Norm of steady state residuals evaluated at each time step*
*15 CV coldplate example*

# RELAXATION FACTOR
## *Optimal Value of ω*

- As the relaxation factor is increased the residuals are driven to zero in fewer iterations
  - ➢ for linear systems $\omega_{Optimal} \approx 1.7$
    - \- an approximate value in linear systems
    - \- can be lower or higher
  - ➢ solution progress can be retarded when ω is outside of optimal as shown

- While there is some ability to predict $\omega_{Optimal}$ for simple problems, it is best to test several values of the relaxation factor when solving the systems
  - ➢ select and apply a value of $\omega$
  - ➢ measure the maximum and sum-total residual after $N_{iterations}$
  - ➢ select ω which gives fastest drop-off rate in the residual

# UNDER-RELAXATION VERSUS OVER-RELAXATION

- Solution stability can be compromised by over-relaxation ω > 1:
  - ➢ **Nonlinear systems**: *may not tolerate over-relaxation and may require under relaxation*
  - ➢ **Example**: *radiation heat transfer, which will be shown to be temperature dependent*
    - effective conductors are temperature dependent
    - may require under-relaxation to maintain solution stability

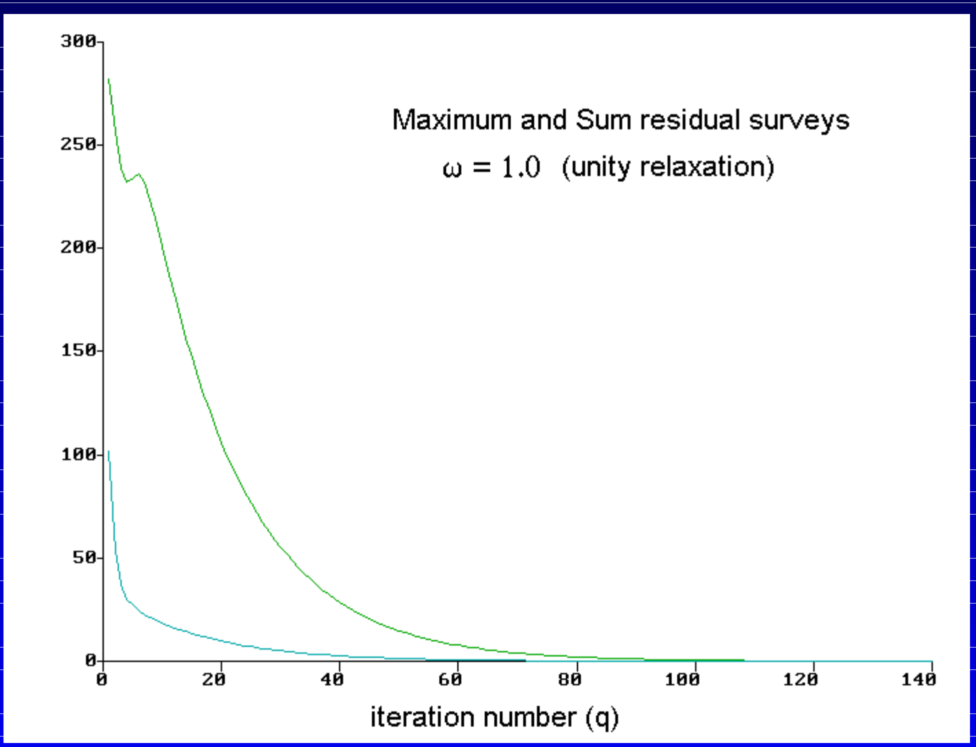
➥ ***It is best to start conservatively by setting ω =1 and then make small changes to optimize the solution efficiency***

# STOPPING CRITERION

## *Assessing the Degree of Steady State*

- We could theoretically iterate the residual equations indefinitely and still observe small updates in the provisional temperature solutions
  - avoid unnecessary iteration by defining a ***termination*** or ***stopping criterion***
  - two approaches generally applied
    - ***residual survey***
    - ***energy survey***

- **Residual Survey**: *terminate when either sum or absolute maximum of φ is less than a user-defined tolerance*
  - *example*: $Max(|\varphi_i|) \leq 0.0001$ then stop iteration
  - *example*: $\sum_{i=1}^{15} |\varphi_i| \leq 0.001$ then stop iteration



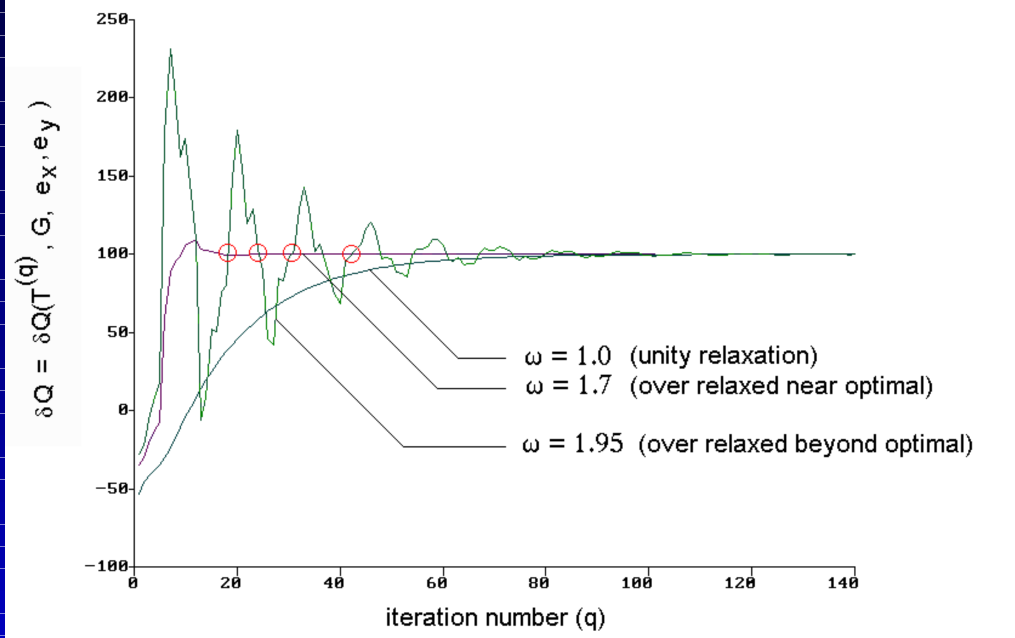

*Residual survey for ω = 1*

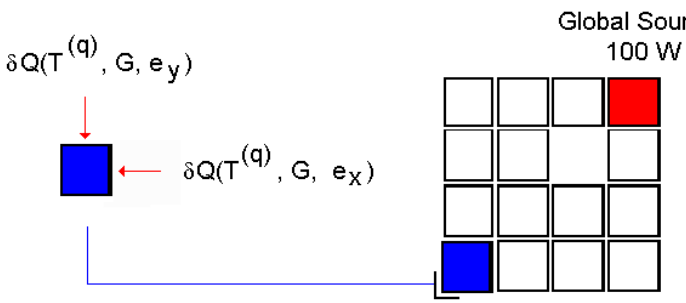
- **Energy Survey**: *terminate when source heating applied to all CV equals the heat flow removed from all boundary CV*

$$\text{example:}\quad \sum_{i=1}^{15} \dot{S}_i - \delta Q(\tilde{T},\ G,\ 1,\ e_{XYZ}) \leq 0.001$$

- Must survey all boundary CV:
  - may be more than just 1 boundary
  - must also include advection term with flow boundaries

- Heat flow added to the boundary CV-1 is oscillatory but should tend naturally to a value of 100 Watts as depicted in figure



Note the cross over point.  This indicates the model is in local balance but only momentarily.  Observe the artificial 2nd order response.  This is discussed below.

**ANIMATION DISPLAY**

Evolution of Steady State Solution - SOR = 1.95

# COMBINING METHODS FOR STOPPING

- A decision based on a localized survey may be faulty
  - ➢ may have energy balance at the inlet and outlet points
    - \- but only momentarily during the progress of the solution
    - \- see crossover points of 100 W line in above figure
  - ➢ iterative solutions can stall and may give the appearance of convergence

- **Hybrid Method**: *use a combination of the 2 residual surveys to establish a stopping criterion and then apply an energy survey as a final check*