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Title: Multidimensional Discrete Ordinates Transport on Massively Parallel Architectures

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Zerr, Robert J.

Intended for: Seminars: U of Florida (2/14/13), Rennselaer Polytech Inst. (3/28/13, U. So. Carolina (4/13)

Multidimensional Discrete Ordinates Transport on Massively Parallel Architectures

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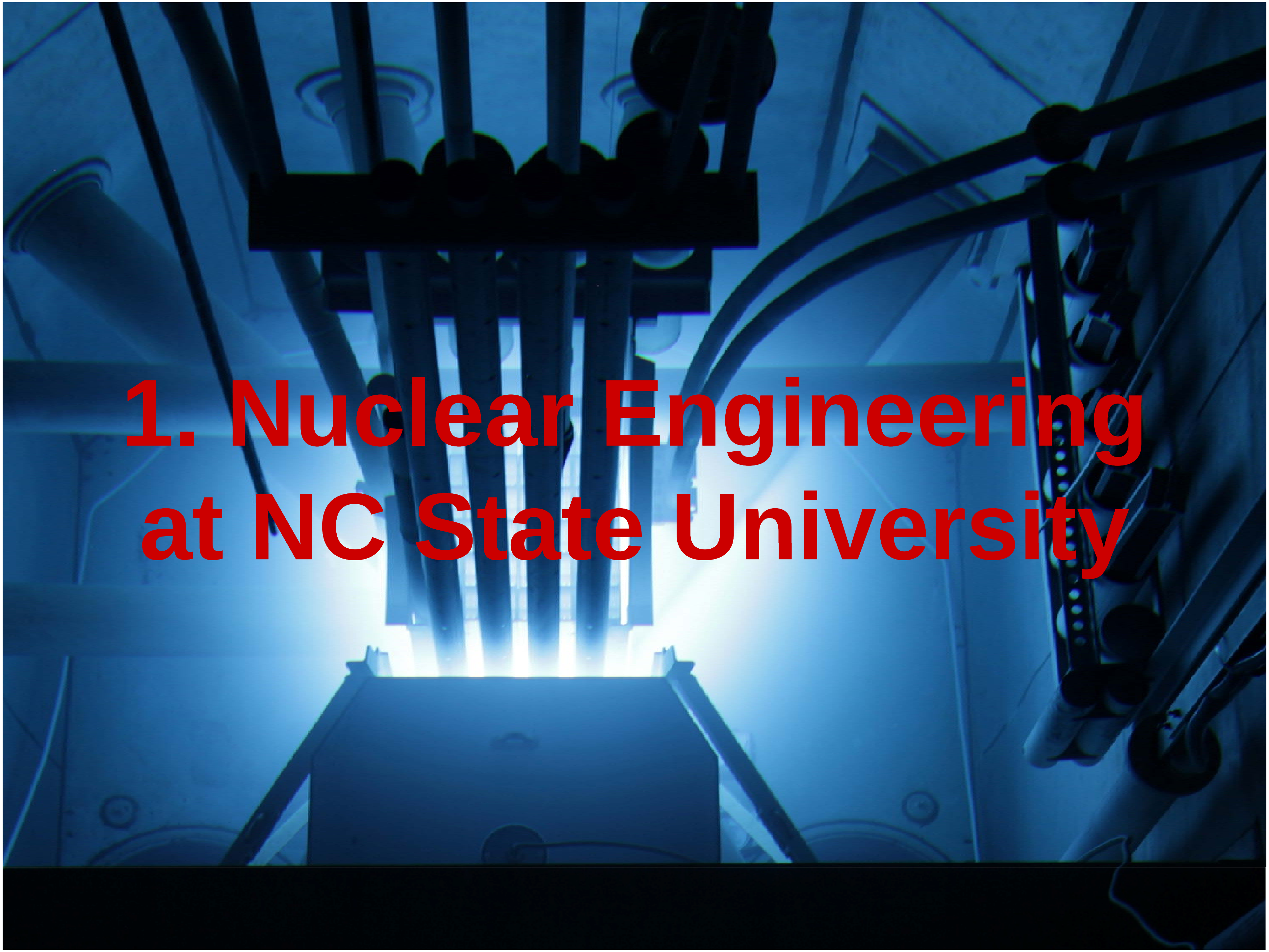
0. Outline



1. Nuclear Engineering at NC State University

1. Department's Brief History

1950 Established as graduate program in Physics Dept

~1950 First non-governmental university-based research reactor

1955 Two PhDs awarded

1962 Department of Nuclear Engineering established

1965 Rapid growth from 4 to 9 faculty; thrust areas: (1) Fission power reactors; (2) Radiation applications

1973 1MW PULSTAR operational (4th on-campus reactor)

1983 Added Plasma/fusion graduate track

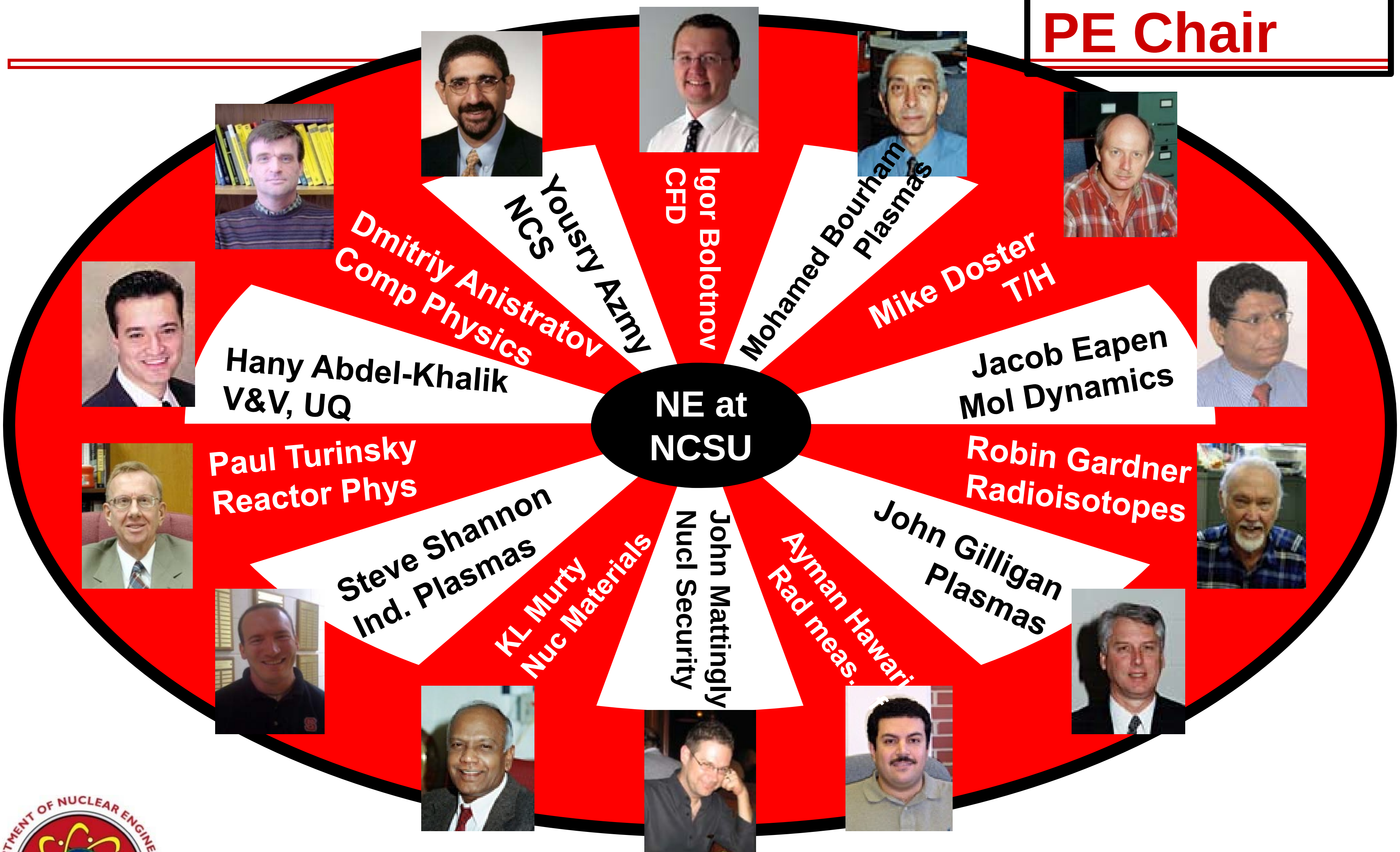
1994 Combined five-year BS/MNE degree established

2008 *Master of Nuclear Engineering* degree via Distance Ed

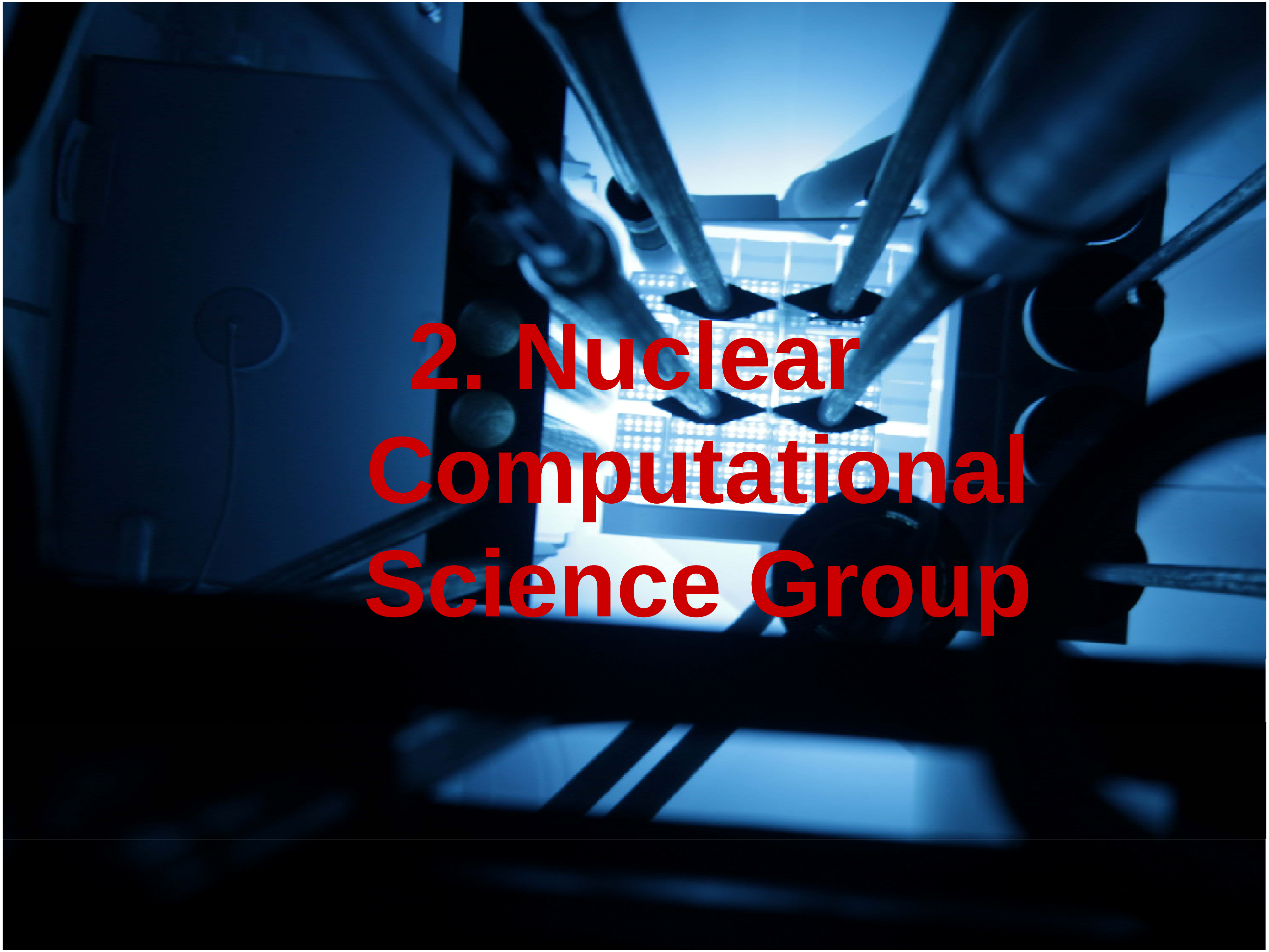
1. NCSU's Nuclear Engineering Today

- **Our Faculty:**
  - 8 active faculty in 2007 ⇨ 15 today
  - 2 open positions currently in search
  - 2 endowed chairs (*Progress Energy* & *Duke Energy*): PE Chair in search
  - Multiple Joint Faculty Appointments with ORNL and INL
  - Pivotal role in CASL: Turinsky Chief Scientist, Doster Ed Programs
  - Gilligan: Director of NEUP
- **Our Students:**
  - Enrolments surpassed 200 UGs & 100 Grads
  - Won Mark Mills Award (best PhD) 9 times in Award's 53 years
  - ~10% win one or more award, scholarship, or fellowship
- **Space:**
  - Increased by more than 50% since 2008
  - Future move to new building on Centennial Campus

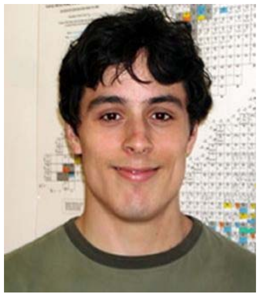
Add Nam & PE Chair



2. Nuclear Computational Science Group



2. NCSG at NCSU



Sebastian Schunert: PhD Student
Thesis: ***Comparing Various Spatial Discretization Schemes Based on a Method of Manufactured Solutions Benchmark Suite***

Sean O'Brien: PhD Student
MS Thesis: A Posteriori ***Error Estimators for the Discrete Ordinates Approximation of the One-Speed Neutron Transport Equation***

Sameer Vhora: MNE Student
Thesis: ***Spectral Analysis of Parallel Block Jacobi Iterations for Solving the Discrete Ordinates Equations with the ITMM Approach***

2. NCSG at NCSU

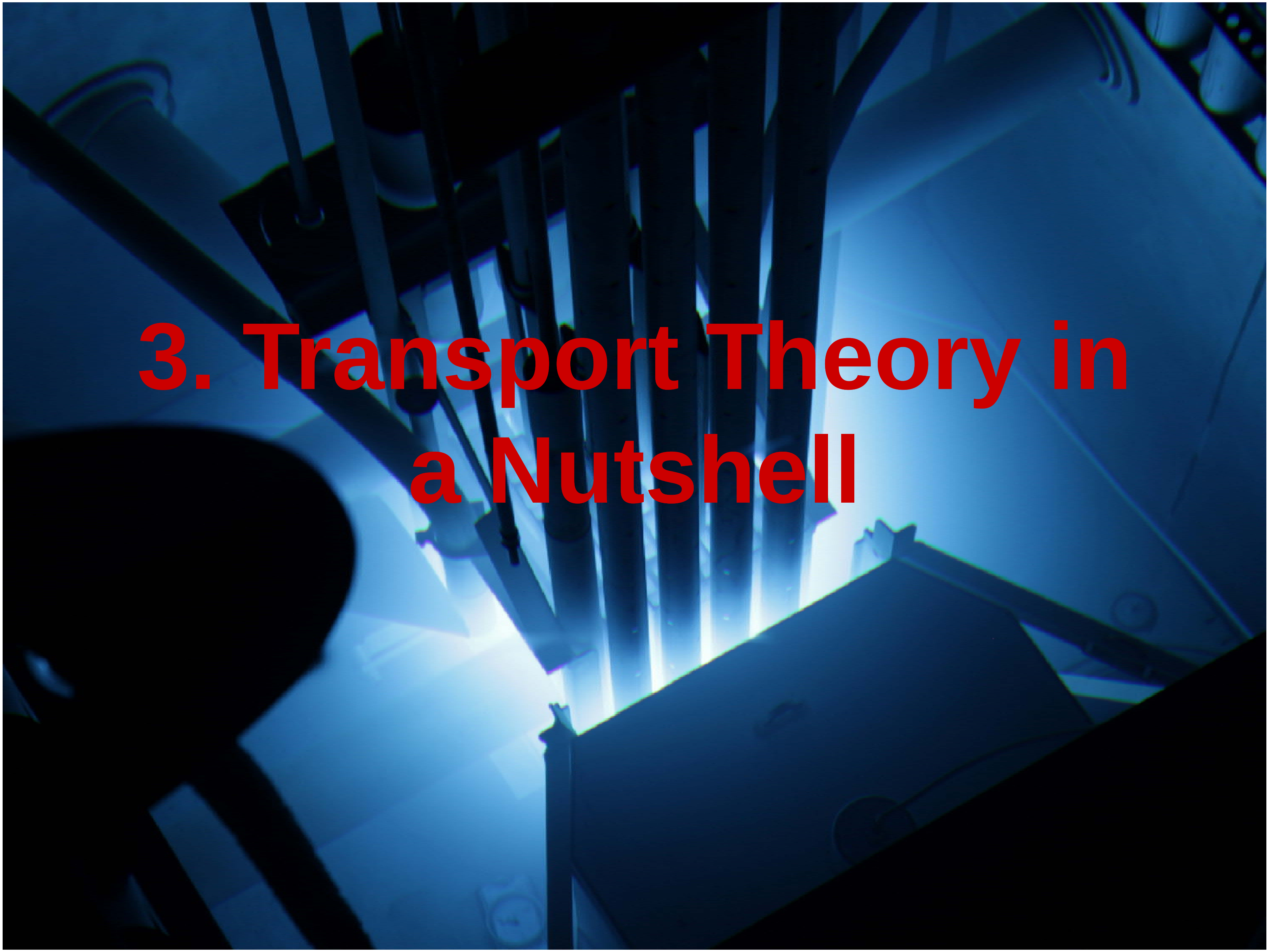
Brian Powell: MS Student
Thesis: ***Efficient Computation of Subdomain Operators Employed in the Integral Transport Matrix Method (ITMM)***

Noel Nelson: MS Student
MS Thesis: ***Accurate Holdup Calculations with Predictive Modeling & Data Integration***

2. Work Presented Today

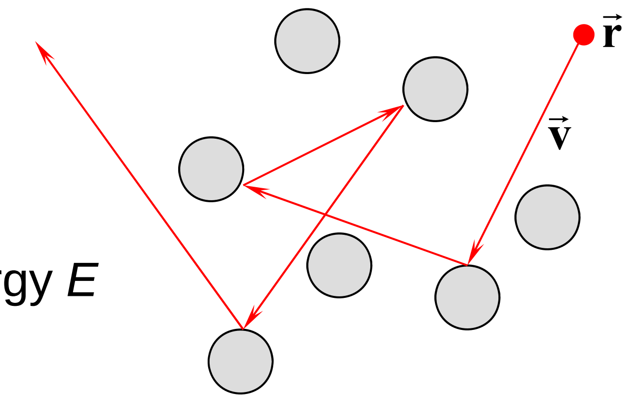
- **Dr. Joe Zerr is a former member of my research group**
- **Presently Research staff at Los Alamos National Laboratory**
- **Received PhD 2010, Penn State University**
- **Recipient of 2010 Mark Mills Award**

3. Transport Theory in a Nutshell



3. Fundamentals

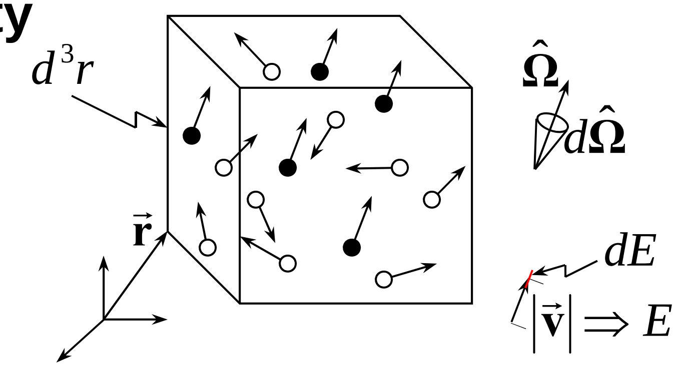
- **Classical point particle is fully described by independent variables:**
  - Time: t
  - Space: $\vec{\mathbf{r}}$
  - Direction of motion: $\hat{\mathbf{\Omega}}$
  - Energy: E
  - **Note**: the unit vector $\hat{\mathbf{\Omega}}$ & energy E are equivalent to velocity $\vec{\mathbf{v}}$



- **Observable quantities (e.g. heating) depend on reaction rate:**
  - Large number of interacting particles (neutrons/photons)
  - Much larger number of host targets (nuclei/electrons)
  - Impractical to solve dynamic system for individual particles/targets ⇨ statistical model: ***mean*** collision density rate
  - Proportional to density of interacting particles & host targets

3. Statistical Model

- **Particle Angular Density:**
  - $n(\vec{\mathbf{r}},\hat{\mathbf{\Omega}},E,t)\,d^3r\,dE\,d\hat{\mathbf{\Omega}} \equiv$ mean number of neutrons at time *t* in d^3r at $\vec{\mathbf{r}}$, with energy in [*E*, *E*+*dE*] traveling in the directional cone $d\hat{\mathbf{\Omega}}$ at $\hat{\mathbf{\Omega}}$
- **Particle Density:**
  - $N(\vec{\mathbf{r}},E,t)\,d^3r\,dE \equiv$ mean number of neutrons at time *t* in d^3r at $\vec{\mathbf{r}}$, with energy in [*E*, *E*+*dE*] ⇨ $N(\vec{\mathbf{r}},E,t) \equiv \int_{4\pi} d\hat{\mathbf{\Omega}}\, n(\vec{\mathbf{r}},\hat{\mathbf{\Omega}},E,t)$
- **Particle Flux: Speed × particle density**
  - Angular flux: $\psi(\vec{\mathbf{r}},\hat{\mathbf{\Omega}},E,t) \equiv vn(\vec{\mathbf{r}},\hat{\mathbf{\Omega}},E,t)$
  - Scalar flux: $\varphi(\vec{\mathbf{r}},E,t) \equiv vN(\vec{\mathbf{r}},E,t)$
  - Leakage rate: $\psi(\vec{\mathbf{r}},\hat{\mathbf{\Omega}},E,t)\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{n}}dA$
  - Reaction rate density: $\Sigma_j\,\varphi(\vec{\mathbf{r}},E,t)$
    - $\Sigma_j \equiv$ Probability reaction *j* / path length



Need to compute $\varphi(\vec{\mathbf{r}},E,t) = \int_{4\pi} \psi(\vec{\mathbf{r}},\hat{\mathbf{\Omega}},E,t)\,d\hat{\mathbf{\Omega}}$

3. Neutron Transport Equation

- **Special case of Boltzmann equation: First-order integro-differential**
  - Neutral particles ⇨ no electro-magnetic forces
  - Low particle densities ⇨ ignore neutron-neutron collisions ⇨ linear
- **Balance over infinitesimal element in phase space:** $(\vec{\mathbf{r}}, \hat{\mathbf{\Omega}}, E)$
- **Dependent variable: Angular flux** $\psi(\vec{\mathbf{r}}, \hat{\mathbf{\Omega}}, E, t)$

$$\underbrace{\frac{1}{v}\frac{\partial \psi(\vec{\mathbf{r}}, E, \hat{\mathbf{\Omega}}, t)}{\partial t}}_{\text{Transient}} + \underbrace{\hat{\mathbf{\Omega}} \cdot \nabla \psi(\vec{\mathbf{r}}, E, \hat{\mathbf{\Omega}}, t)}_{\text{Streaming}} + \underbrace{\Sigma_t(\vec{\mathbf{r}}, E)\psi(\vec{\mathbf{r}}, E, \hat{\mathbf{\Omega}}, t)}_{\text{Total collision}}$$

$$\text{Scattering}\left\{ = \int_{4\pi} d\hat{\mathbf{\Omega}}' \int_0^\infty dE' \Sigma_s(E', \hat{\mathbf{\Omega}}' \to E, \hat{\mathbf{\Omega}}) \psi(\vec{\mathbf{r}}, E', \hat{\mathbf{\Omega}}', t) \right.$$

$$\text{Fission}\left\{ + \frac{\chi(E)}{4\pi}\left[\int_0^\infty dE' \nu(E') \Sigma_f(\vec{\mathbf{r}}, E') \int_{4\pi} d\hat{\mathbf{\Omega}}' \psi(\vec{\mathbf{r}}, E', \hat{\mathbf{\Omega}}', t)\right] \right. + \underbrace{s(\vec{\mathbf{r}}, E, \hat{\mathbf{\Omega}}, t)}_{\text{Fixed source}}$$

3. Interface & Boundary Conditions

- **Steady state: Time derivative vanishes**
- **Interface condition: Angular flux continuous along direction of motion, $\hat{\mathbf{\Omega}}$, across material boundaries**
- **Physical intuition: Can specify what goes into a system**
  - What comes out is a consequence of the transport process inside
  - Example: shining light into crystal
    - Can choose color/intensity of incoming light
    - Can't choose color/intensity of outgoing light: depends on what happens inside
- **Typical Boundary Condition (BC):**
  - Set ***incoming*** flux $\psi(\vec{\mathbf{r}}_s, E, \hat{\mathbf{\Omega}}, t) = \psi_{in}(\vec{\mathbf{r}}_s, E, \hat{\mathbf{\Omega}}, t)$ for:
    - All times *t*
    - All energies: $E \in [0, \infty]$
    - Each $\vec{\mathbf{r}}_s$ on the boundary *S*
    - Each incoming angle: $\hat{\mathbf{\Omega}} \cdot \hat{\mathbf{e}}_s < 0, \hat{\mathbf{e}}_s$ is the normal unit vector pointing out
  - The function $\psi_{in}(\vec{\mathbf{r}}_s, E, \hat{\mathbf{\Omega}}, t)$ can be specified explicitly or implicitly
    - Vacuum BC: $\psi_{in}(\vec{\mathbf{r}}_s, E, \hat{\mathbf{\Omega}}, t) = 0$

3. Discretization of Transport Equation

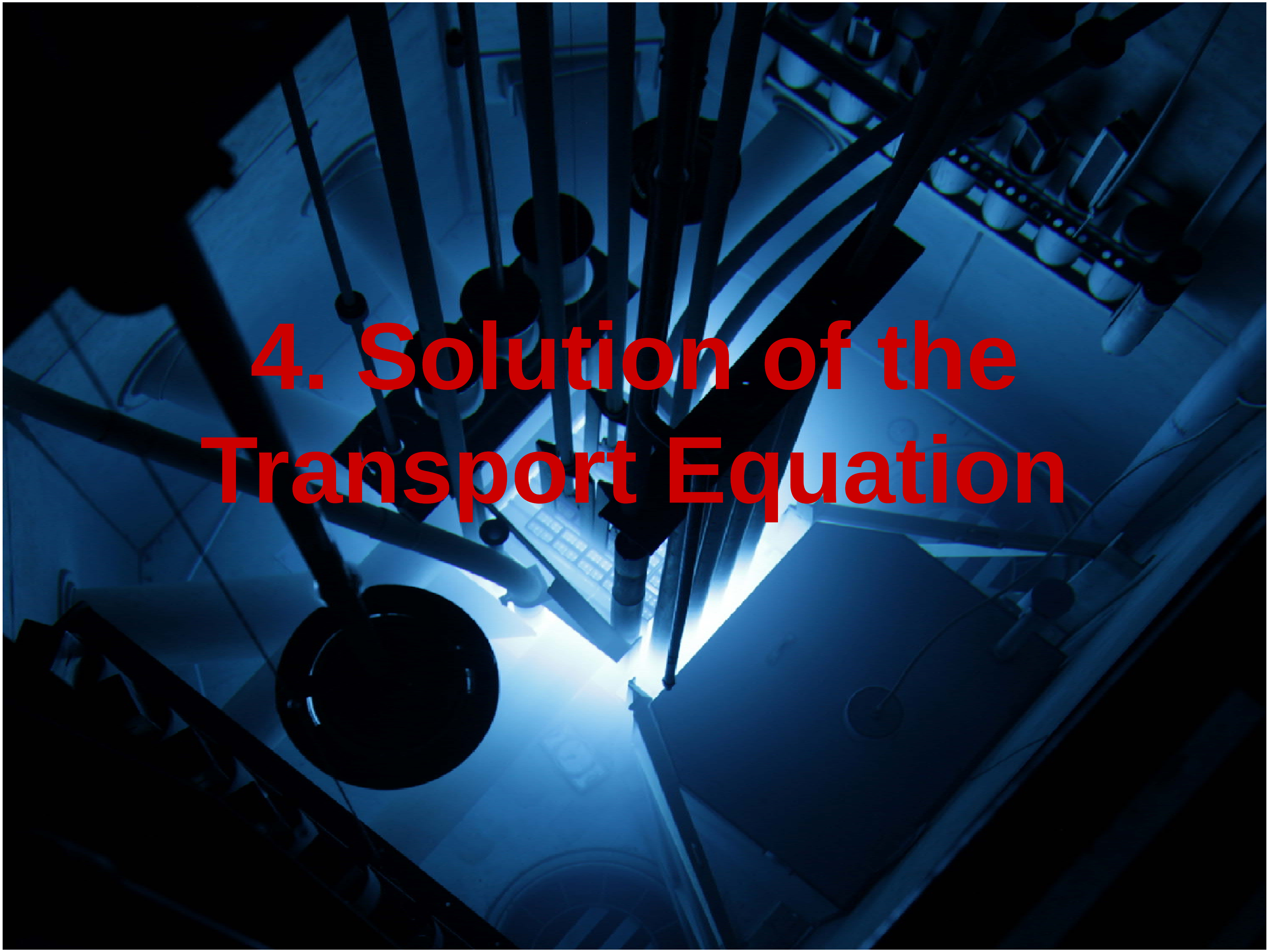
- ❑ **Implementation on digital computer ⇨ discretize independent variables & consequently dependent variables**
- ❑ **Energy: Multigroup ⇨ discretization into *bins* (E_g , E_{g-1})**
  - ❖ Victory, 1985: Total & scattering cross section fluctuations diminish with refinement of energy group structure

    ⇨ Multigroup solution → exact solution
- ❑ **Angle: Discrete-ordinates ⇨ discretization along discrete $\hat{\Omega}_n$**
  - ❖ Madsen, 1971: Quadrature formula converges with increasing order

    ⇨ Discrete Ordinates solution → exact one-speed solution
- ❑ **Space: Multitude of methods discretize $\nabla\psi$ on spatial mesh**
  - ❖ Madsen, 1972: Exact solution has bounded 3rd derivatives

    ⇨ Diamond Difference solution → exact Discrete Ordinates solution
  - ❖ Smoothness hypothesis unrealistic for most applications

4. Solution of the Transport Equation



4. Traditional Solution Algorithms

- **Difficulty of solving the transport equation (partial list):**
  - Steady-state 3-D problems: phase space is 6-D ⇨ 100 discrete variables per phase space dimension yields 10^{12} unknowns
  - Neutron cross sections sensitive to energy & nuclide composition
  - Source (fission & scattering) depends on solution ψ ⇨ iterate
- **Nested loops:**
  - Outer Iteration: converge fission/scattering source
  - Loop over energy groups: from highest to lowest *E*
  - In each group sum fission + inscattering source guess into *q*
  - Inner (or Source) Iteration: reconcile within group source & flux
    - Starting with guess for group φ within-group scattering source
    - Invert 1^{st} order PDE on source distribution ⇨ group ψ
    - Integrate over angle ⇨ new φ: test if too different from starting guess
    - Yes: Repeat unless already used too many iterations
    - No: solution converged successfully to group flux for into-group sources

4. Cell Equations

- **Kernel operation: Solving 1st order PDE for given source**
  - Conducted via *mesh sweep* algorithm: 1 cell, 1 angle at a time
- **Discretized equations per energy group/angle/cell:**
  - Balance: Include fission & inscattering from other groups in q_n

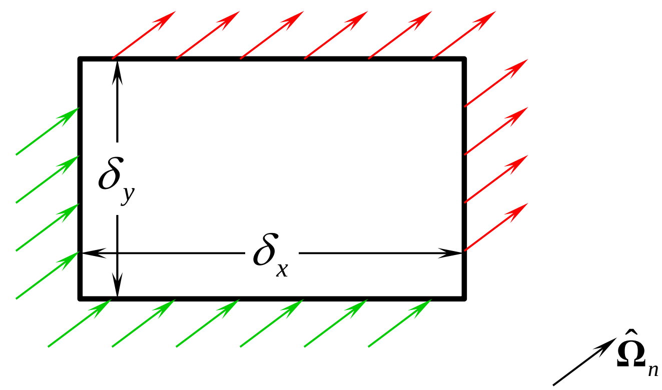
$$\frac{\mu_n}{\delta_x}\left(\psi^x_{n,out}-\psi^x_{n,in}\right)+\frac{\eta_n}{\delta_y}\left(\psi^y_{n,out}-\psi^y_{n,in}\right)+\frac{\xi_n}{\delta_z}\left(\psi^z_{n,out}-\psi^z_{n,in}\right)+\sigma_t\,\overline{\psi}_n=\sigma_s\,\overline{\varphi}+q_n$$

  - Auxiliary: Method-dependent, simplest is Diamond Difference

$$\overline{\psi}_n=\frac{1}{2}\left(\psi^u_{n,out}+\psi^u_{n,in}\right),\quad u=x,y,z$$

  - Quadrature formula:

$$\overline{\varphi}=\sum_{n=1}^{N}\omega_n\overline{\psi}_n$$



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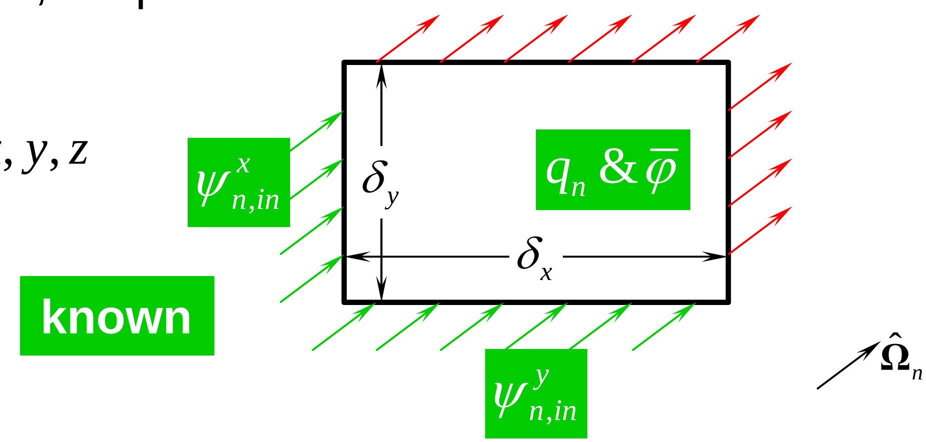

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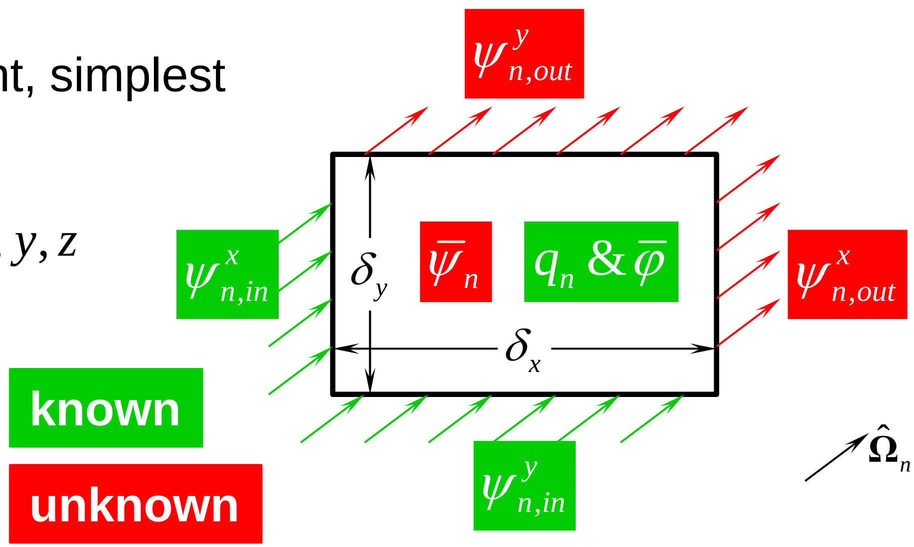
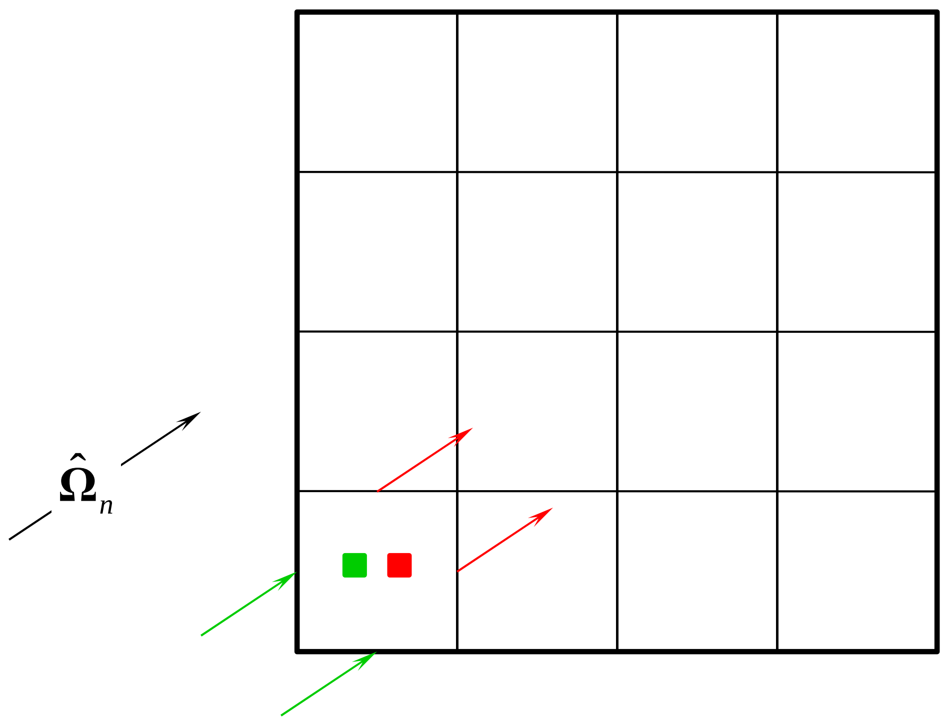


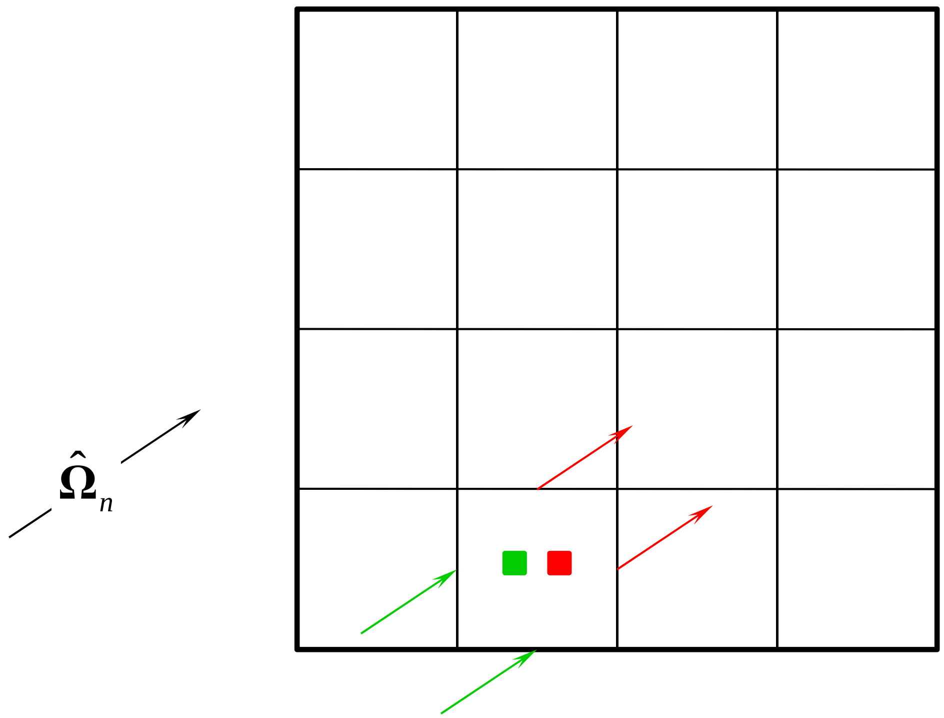
4. Mesh Sweep

- **For each discrete ordinate sweep cells along $\hat{\Omega}_n$**



4. Mesh Sweep

- Interface angular fluxes couple neighboring cells



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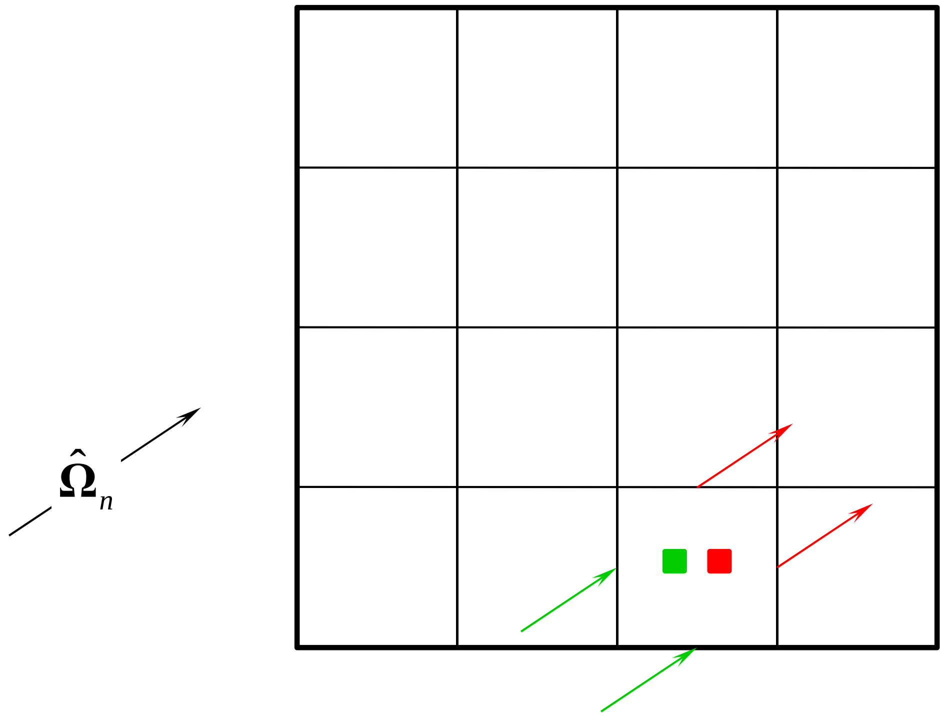
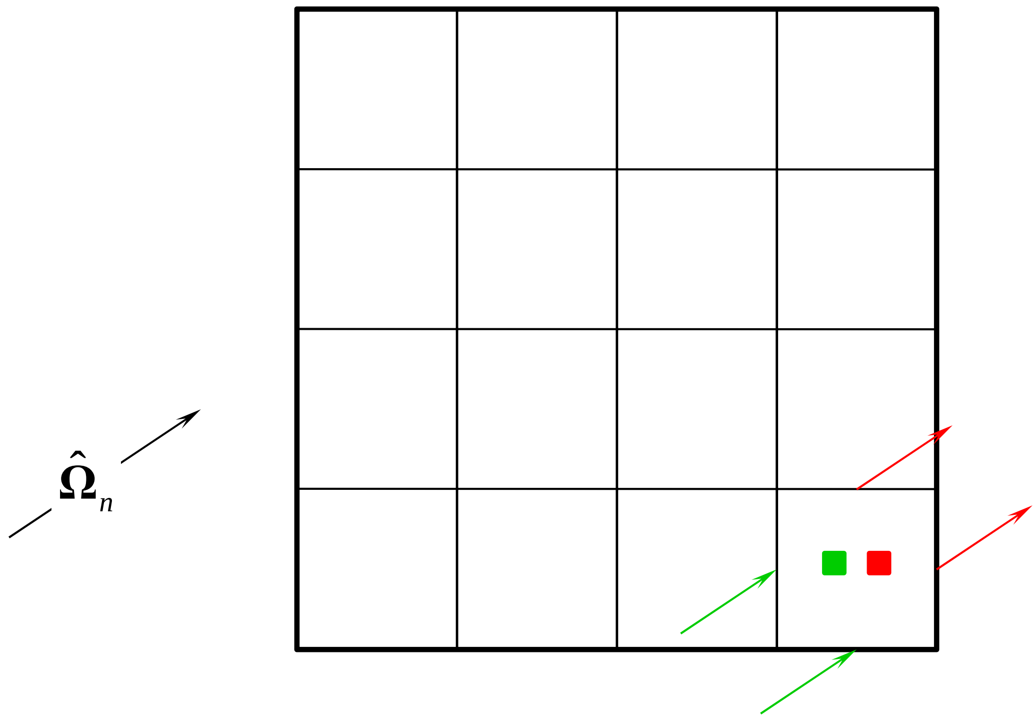


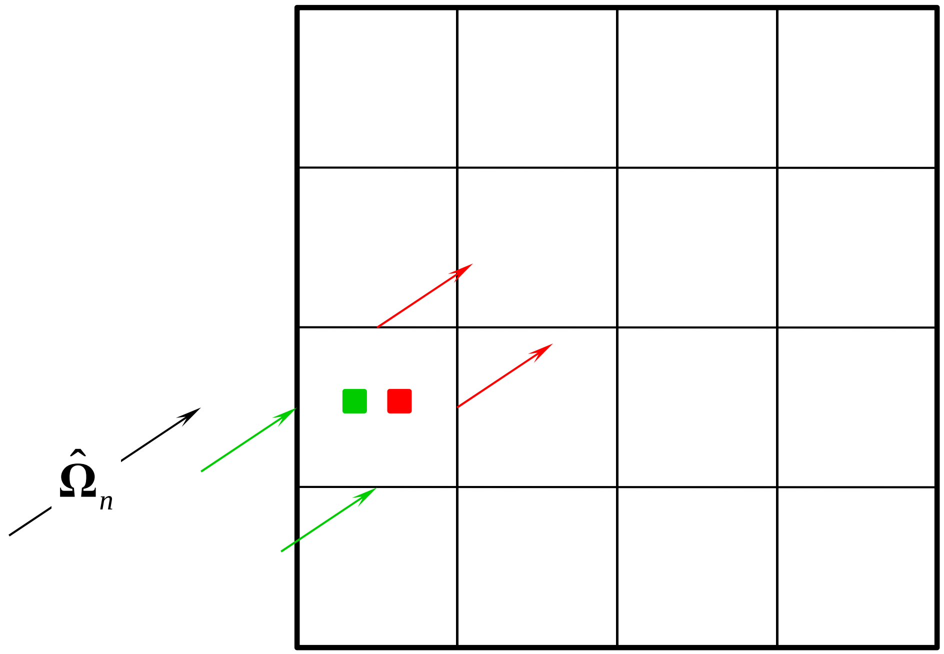
4. Mesh Sweep

- **Upon reaching end of row go to next row along $\hat{\Omega}_n$**



4. Mesh Sweep

- ❑ **Note sequential nature: must compute upstream cell first**



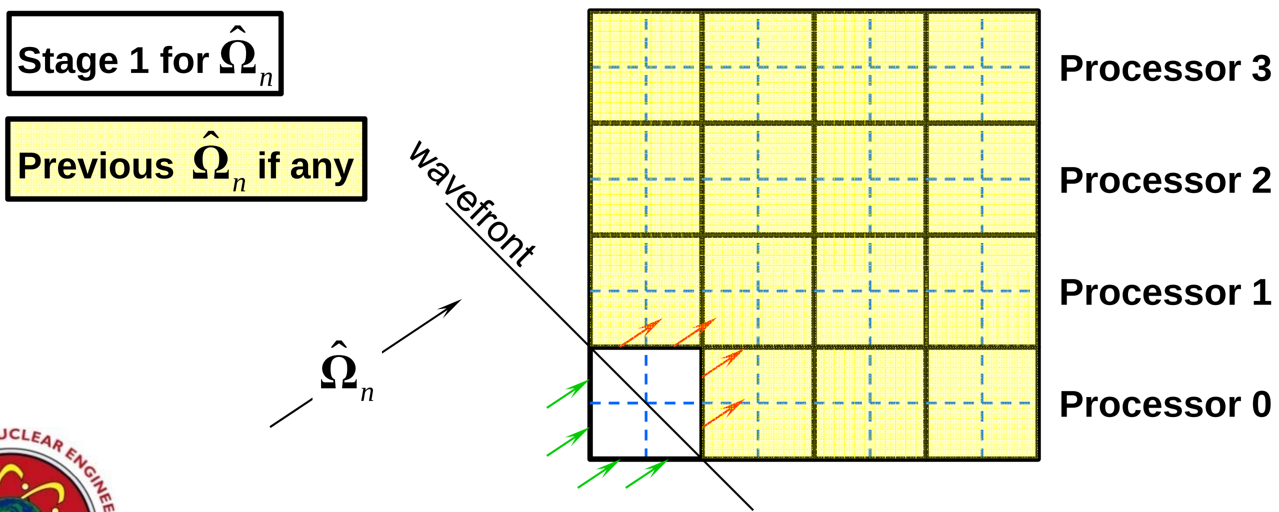
- ❑ **Slow convergence if SI often demands acceleration (DSA)**

4. Parallelization Strategies

- ***Domain decomposition*: split range of phase space variable in *P* subdomain & assign each to different process**
  - Perfect parallelization ⇨ reduce execution time by factor *P*
  - ***Synchronous*** DD: processes fully independent ⇨ computation (e.g. number of iterations) independent of *P*
  - ***Asynchronous*** DD: coupled processes ⇨ work *P* dependent
- **Possible DD for S_N algorithms:**
  - Energy: speedup limited by # groups (hundreds at most)
    - Coarse-grain ⇨ easy to implement & high parallel efficiency
    - Asynchronous & pointless unless there is fission &/or upscattering
  - Angle: speedup limited by # angles (few thousands at most)
    - Medium-grain ⇨ easy to implement & good parallel efficiency
    - Synchronous in Cartesian coordinate system
  - Spatial: speedup limited by # cells (potentially many millions)
    - Fine-grain ⇨ difficult to implement & OK parallel efficiency
    - Synchronous implies retaining sequential order among subdomains

4. Spatial Domain Decomposition

- **Koche- Baker-Alcouffe SDD: synchronous**
  - Maps 3D mesh onto 2D processor topology
  - Sweep mesh by subdomain in natural sequence per $\hat{\mathbf{\Omega}}_n$
  - Concurrently sweep ready subdomains (on waverfront) ➪ SDD
  - Pipeline angles to reduce processor idleness
  - Communicate outgoing interface ψ to neighbors across wavefront



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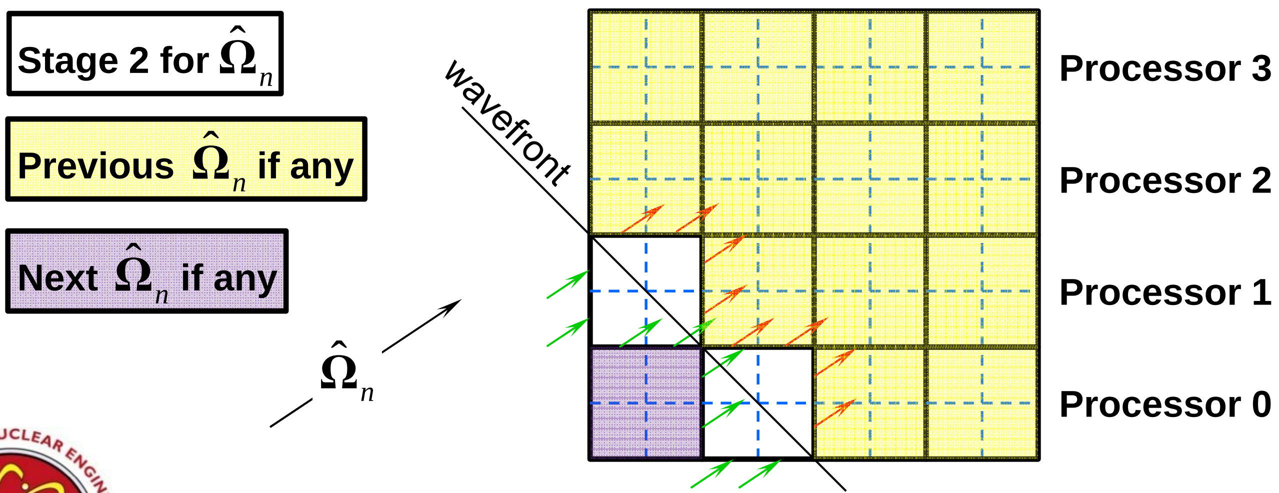
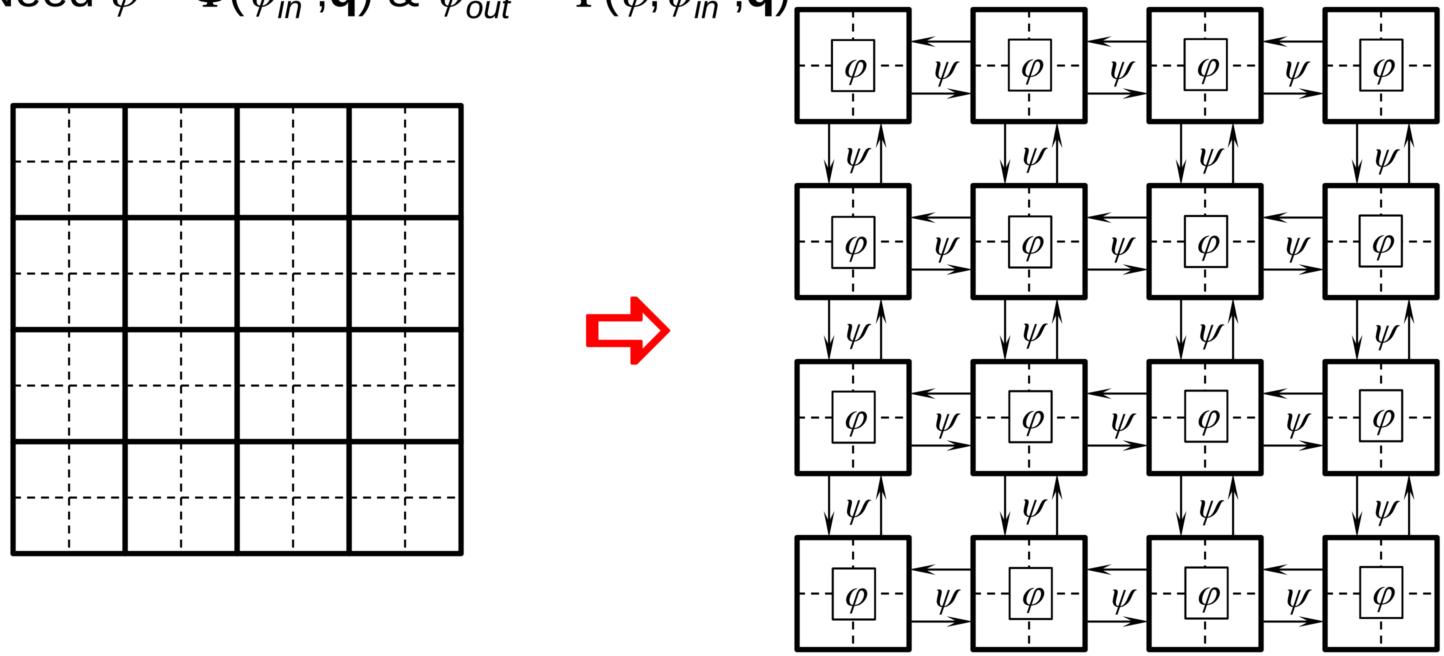


5. Alternative SDD Parallelizations

5. Parallel Block Jacobi (PBJ)

- **Asynchronous SDD alternative to KBA:**
  - Eliminate processor idleness & increase concurrent processes
  - Combine all angles computations in subdomain via ITMM operators
  - Replace SI with iterations on subdomain interface fluxes: Communicate ψ between iterations
  - Need $\varphi = \Phi(\psi_{in}, \mathbf{q})$ & $\psi_{out} = \Psi(\varphi, \psi_{in}, \mathbf{q})$



5. Outline of ITMM

- **Express SI as a mapping of flux ℓ iterate into ℓ+1 iterate:**

$$\varphi^{(\ell+1)} = \mathbf{J}_\varphi \left(\varphi^{(\ell)} + \Sigma_s^{-1} \mathbf{q} \right) + \mathbf{K}_\varphi \psi_{in} \quad \Rightarrow \quad \mathbf{J}_\varphi = \partial \varphi^{(\ell+1)} \big/ \partial \varphi^{(\ell)}$$

  - Upon iterative convergence:

$$\left(\mathbf{I} - \mathbf{J}_\varphi \right) \varphi^\infty = \mathbf{J}_\varphi \Sigma_s^{-1} \mathbf{q} + \mathbf{K}_\varphi \psi_{in} \quad \rightarrow \quad \mathbf{\Phi}\left(\psi_{in}, \mathbf{q} \right)$$

  - For full domain where ψ_{in} is known from BCs:

$$\psi_{out} = \mathbf{J}_\psi \left(\varphi^\infty + \Sigma_s^{-1} \mathbf{q} \right) + \mathbf{K}_\psi \psi_{in} \quad \rightarrow \quad \mathbf{\Psi}\left(\varphi, \psi_{in}, \mathbf{q} \right)$$

- **Apply to subdomain: ψ_{in} is not known requires iteration**

- **ITMM operators are response matrices:**
  - $\mathbf{J}_\varphi$: cell-averaged scalar flux due to unit distributed source
  - $\mathbf{K}_\varphi$: cell-averaged scalar flux due to unit incident angular flux
  - $\mathbf{J}_\psi$: outgoing angular flux due to unit distributed source
  - $\mathbf{K}_\psi$: outgoing angular flux due to unit incident angular flux

5. Construction of ITMM Operators

- **Differential Mesh Sweep (DMS): concurrently in all subdomains**
  - Perform single sweep to compute elements of $\mathbf{J}_\varphi$ via $\mathbf{J}_\varphi = \partial\varphi^{(\ell+1)} / \partial\varphi^{(\ell)}$
  - Compute elements of other operators along the way

- **Dense operators: memory limitations as size grows**
  - Operators sizes grow superlinear with # cells, linear with # angles
  - Full coupling of cell- and face-fluxes
  - Expensive to invert for large subdomains

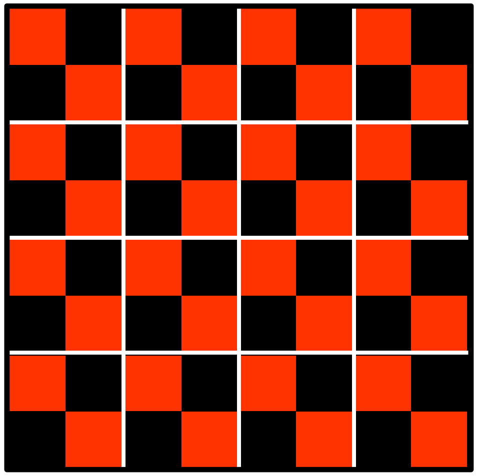
- **Applicable to high-order spatial discretizations & anisotropic scattering (φ ⇨ angular moments)**

5. PBJ Algorithm

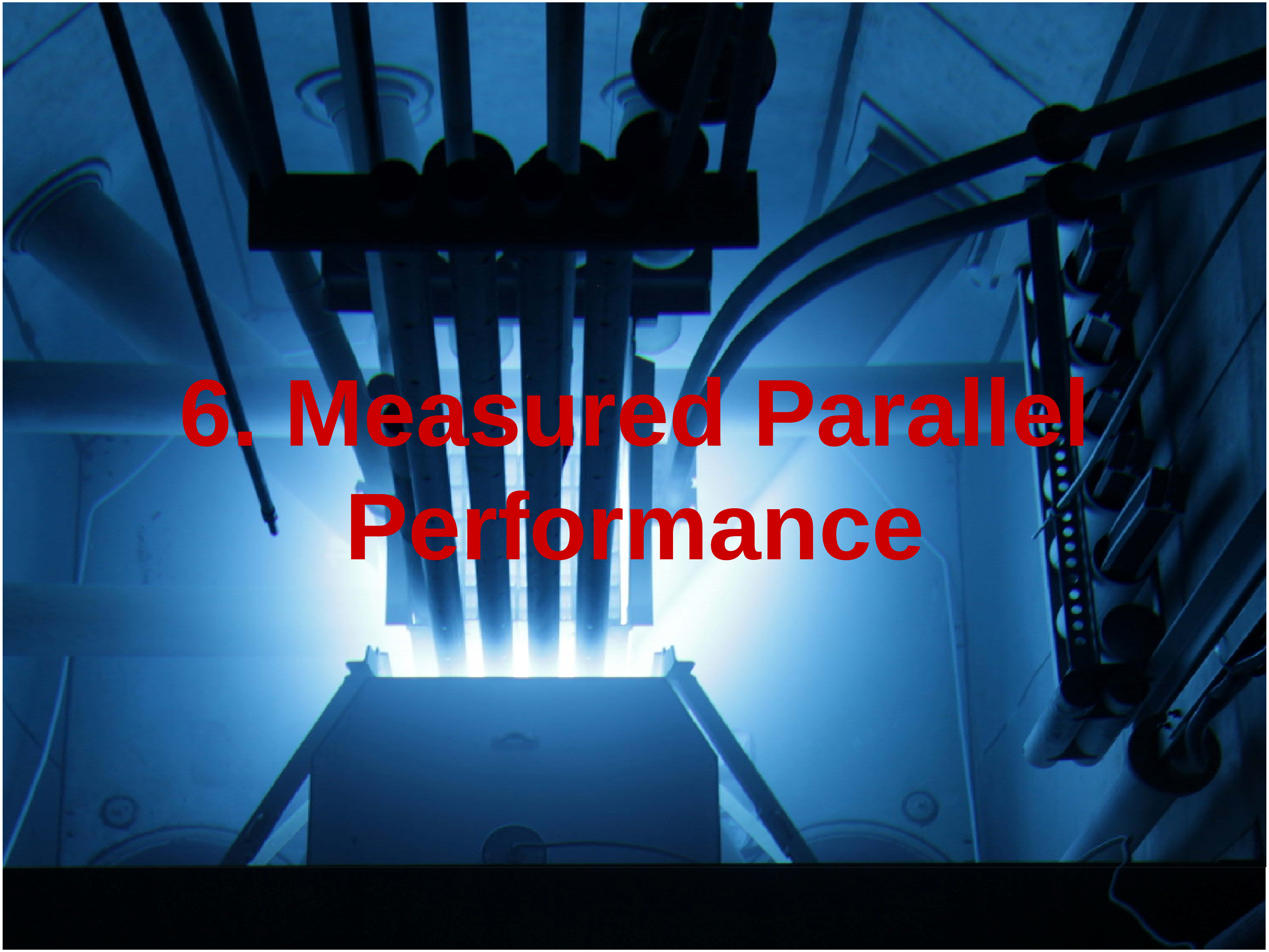
- **For each energy group, fully concurrent:**
  - Perform DMS per subdomain/processor ⇨ 4 ITMM operators
  - Need to effect $(\mathbf{I}-\mathbf{J}_{\varphi})^{-1}$ ⇨ LU factorization only once then store
  - Execute PBJ iterations on subdomain interface angular fluxes:
    - Given $\psi_{in}^{(\lambda)}$ compute for each subdomain $\varphi^{(\lambda+1)} = \mathbf{\Phi}\left(\psi_{in}^{(\lambda)}, \mathbf{q}\right)$
    - Test convergence of scalar flux: $\left|1-\varphi^{(\lambda+1)}/\varphi^{(\lambda)}\right|$ small?
      - If converged go to next group (if any)
      - Otherwise start new iteration with: $\psi_{out}^{(\lambda+1)} = \mathbf{\Psi}\left(\varphi^{(\lambda+1)}, \psi_{in}^{(\lambda)}, \mathbf{q}\right)$
      - Communicate $\psi_{out}^{(\lambda+1)}$ as $\psi_{in}^{(\lambda+1)}$ to neighboring subdomains
- **Observations:**
  - Reduced local computations to matrix-vector multiplies & adds
  - Sources of parallel inefficiency:
    - Increasing # iterations with *P* & tighter subdomain coupling: *c*↑ & Σ_t *h*↓
    - Network contention: Communicate subdomain interface angular fluxes

5. Parallel Gauss-Seidel (PGS)

- **Red/Black splitting of each subdomain:**
  - Each sub-subdomain is either **red** or **black**
  - Operations per global iteration over interface angular flux:
    - Solve local ITMM system for φ & ψ_{out}
    - Copy/send $\psi_{out} \rightarrow \psi_{in}$ to intra-/iter-subdomain neighbor
    - Solve local ITMM system for φ & ψ_{out}
    - Copy/send $\psi_{out} \rightarrow \psi_{in}$ to intra-/iter-subdomain neighbor
  - Pros:
    - Memory requirement ↓ super-linearly with ↓ number of cells
    - Typically Gauss-Seidel convergence rate better than Block Jacobi
  - Cons:
    - Smaller ITMM subdomains ⇨ slower convergence of global iterations



6. Measured Parallel Performance

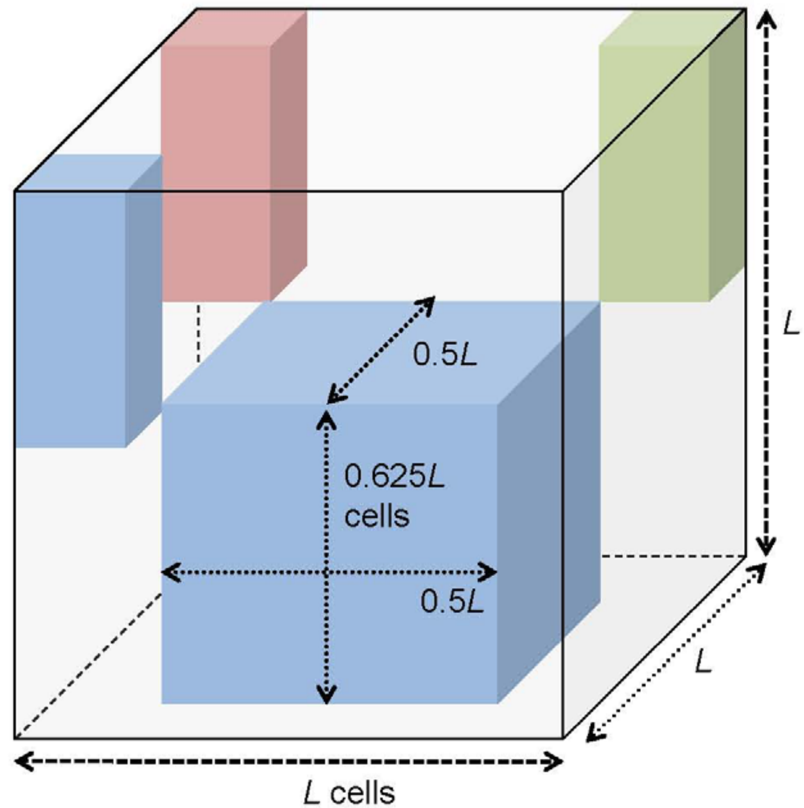


6. Implementation in PIDOTS

- **Implemented PBJ & PGS in *Parallel Integral Discrete Ordinates Transport Solver* (PIDOTS)**
- **All tests performed with one-group, DD, with isotropic scattering**
- **Preliminary testing on:**
  - LANL's Yellowrail:
    - 139 compute nodes each with 8 Processing Elements (PE) & 16 GB memory
    - Runs up to P = 256 processes
  - LANL's Redtail:
    - 1,834 compute nodes each with 8 PEs & 32 GB memory
    - Runs up to P = 1,024
  - ORNL's JaguarPF: All results here are for this platform
    - 18,688 compute nodes each with 12 PEs & 16 GB memory
    - Runs up to P = 32,768

6. Weak Scaling Tests

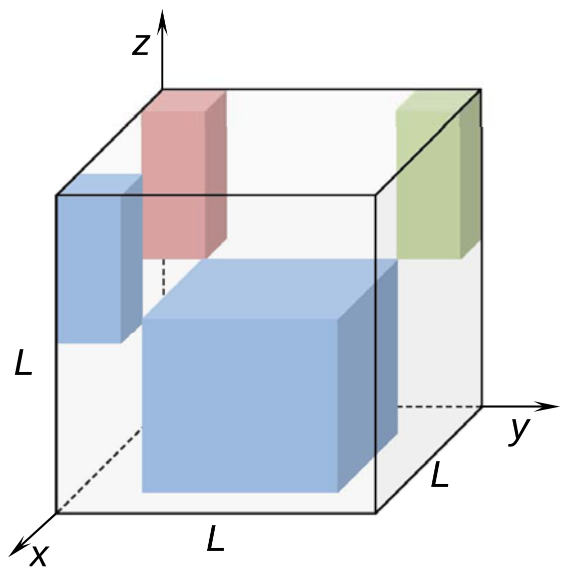
- **Evaluate parallel performance as problem size grows with *P***
- **Weak scaling ⇨ Number of cells per processor fixed:**
  - Start with *L* x *L* x *L* cubic-cells domain
  - Comprised of 4 materials: no symmetries
  - Examine effect on number of iterations ⇨ execution time:
    - Cell size *h* set to {0.1, 1.0, 10.0} cm
    - Scattering ratio *c* set to {0.9, 0.99}
  - Choice of *L* & S_N order is memory-limited



Dept of Nuclear Engineering
NC State University

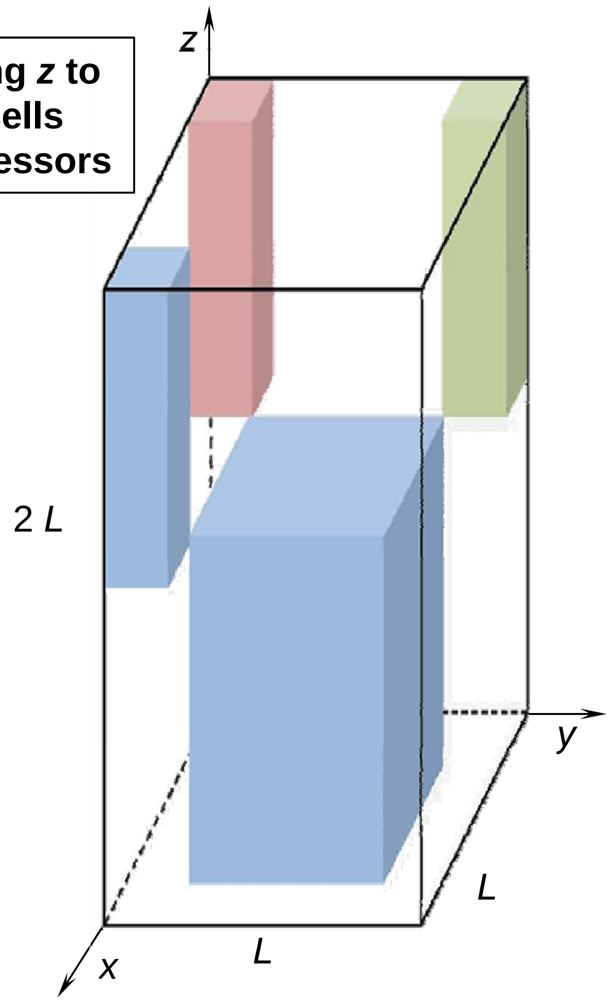
6. Growing Problem Size

Starting with the base case:
***L* x *L* x *L* cells**
on *P* processors



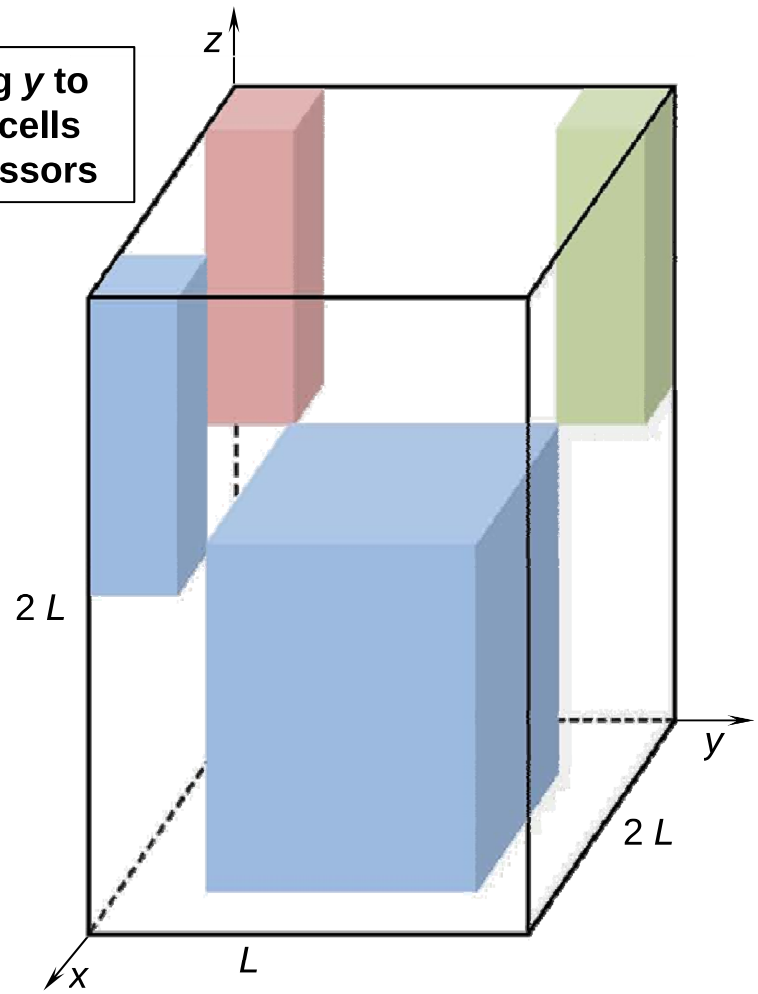
6. Growing Problem Size

Stretch along *z* to
***L* x *L* x 2 *L* cells**
on 2 *P* processors



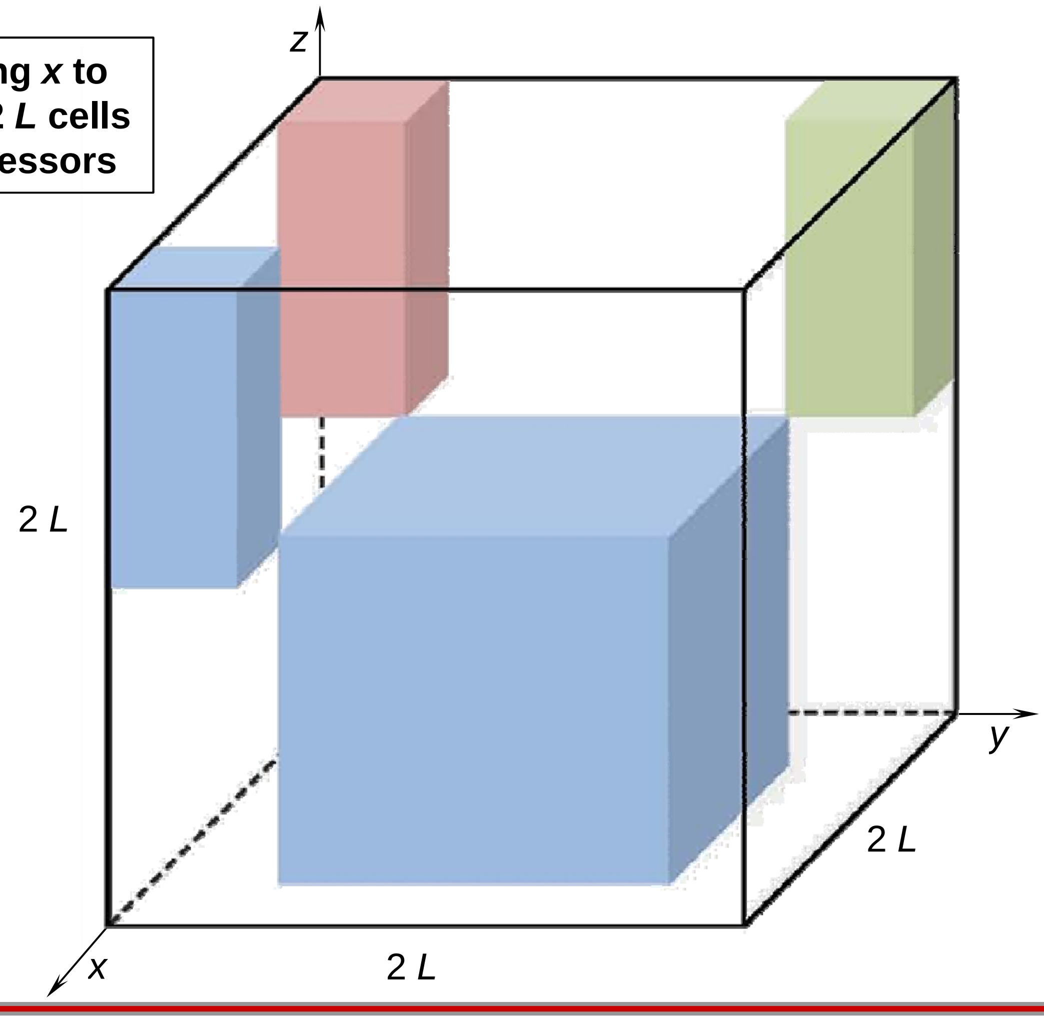
6. Growing Problem Size

Stretch along *y* to *L* x 2 *L* x 2 *L* cells on 4 *P* processors



6. Growing Problem Size

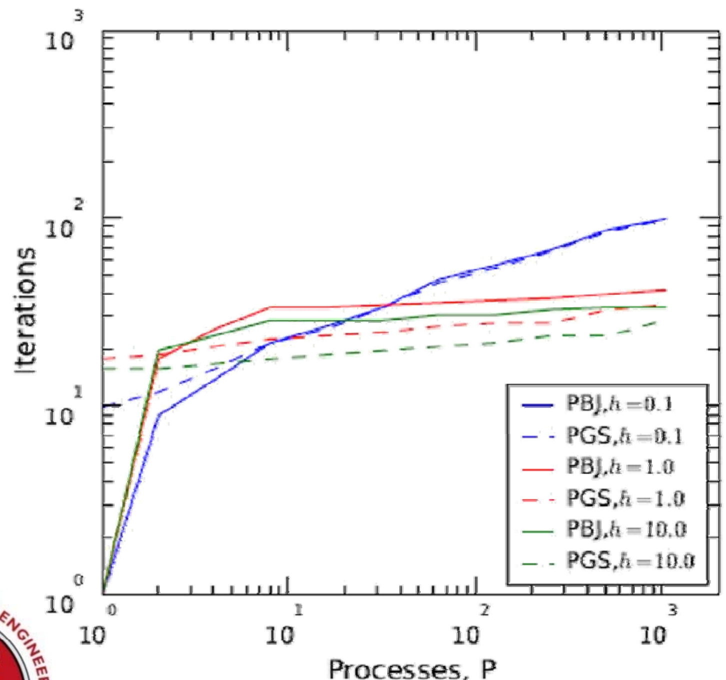
Stretch along *x* to
2 *L* x 2 *L* x 2 *L* cells
on 8 *P* processors

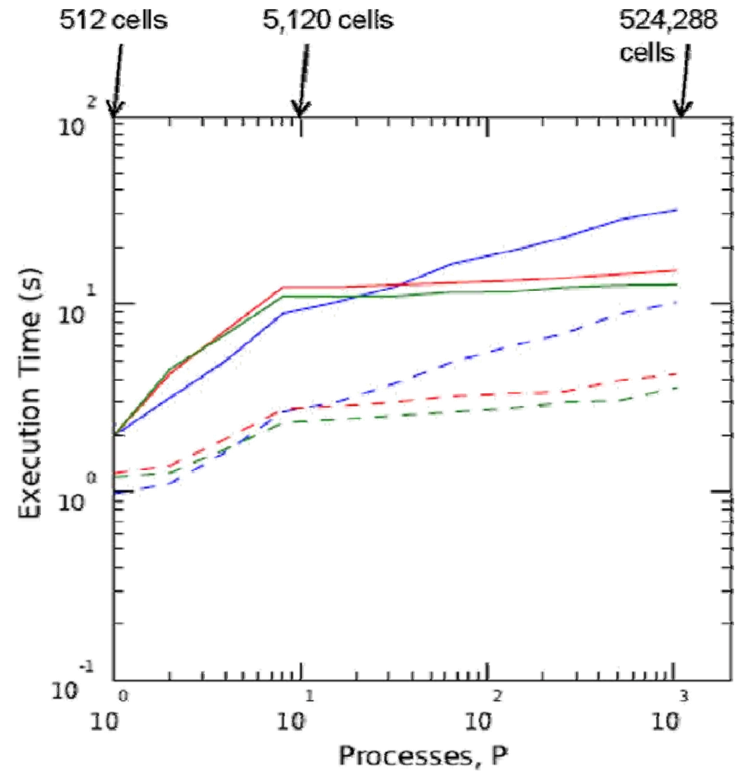


6. PBJ *vs* PGS Performance

- **8x8x8-cell model per *P*, S_{16}, *P* up to 1,024 on JaguarPF**
- **PGS: eight 4x4x4-cell sub-subdomains per *P* ⇨ shorter construction & per-iteration times**

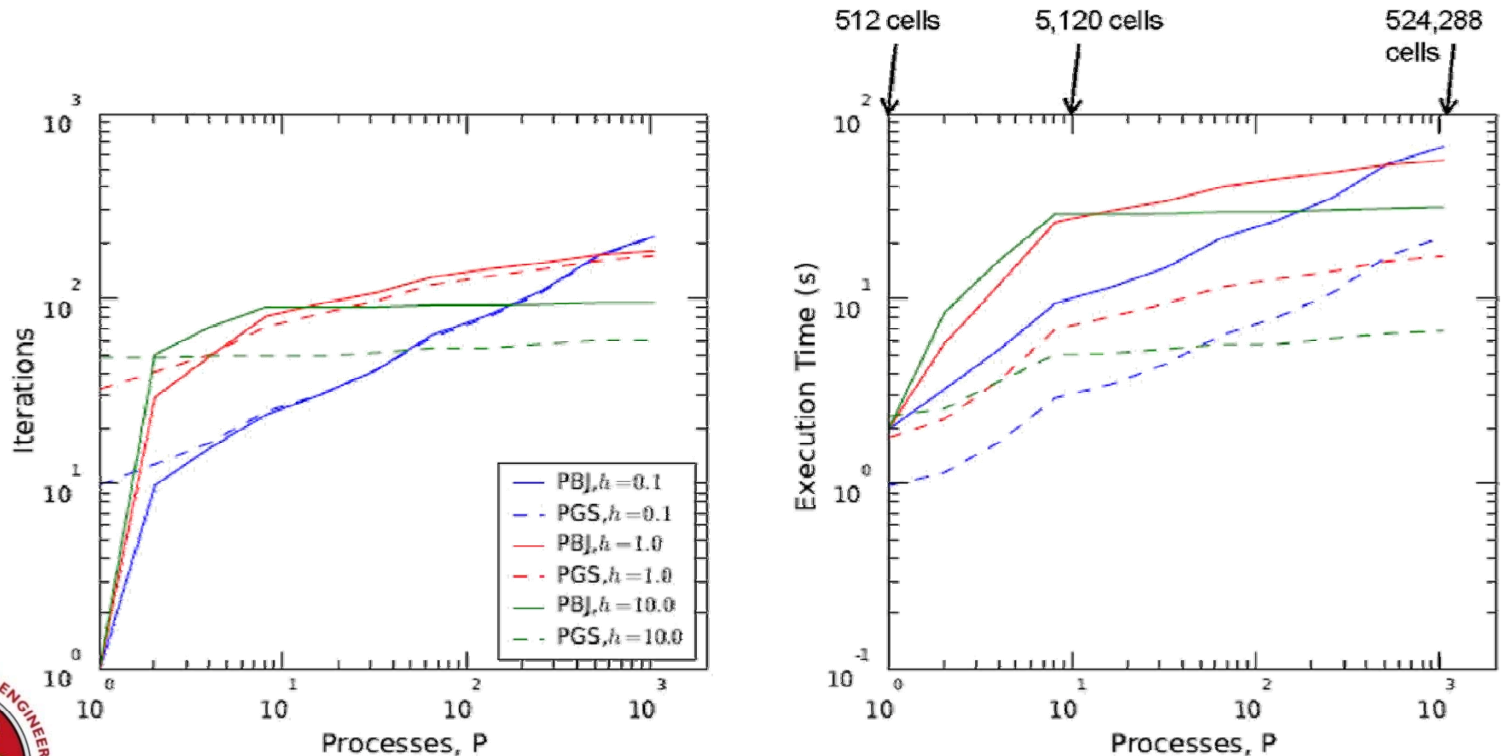
c = 0.9 results:





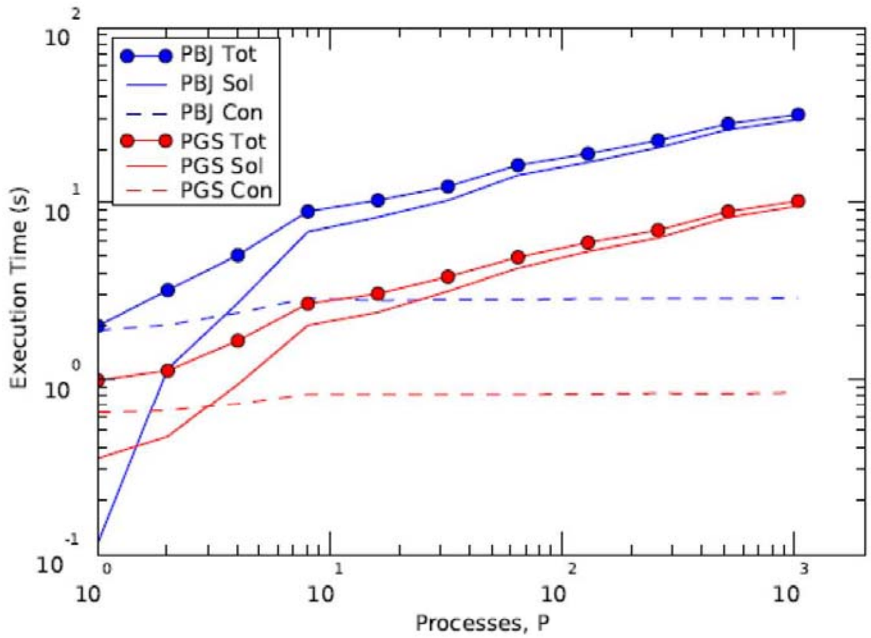
6. PBJ *vs* PGS Performance

c = 0.99 results:



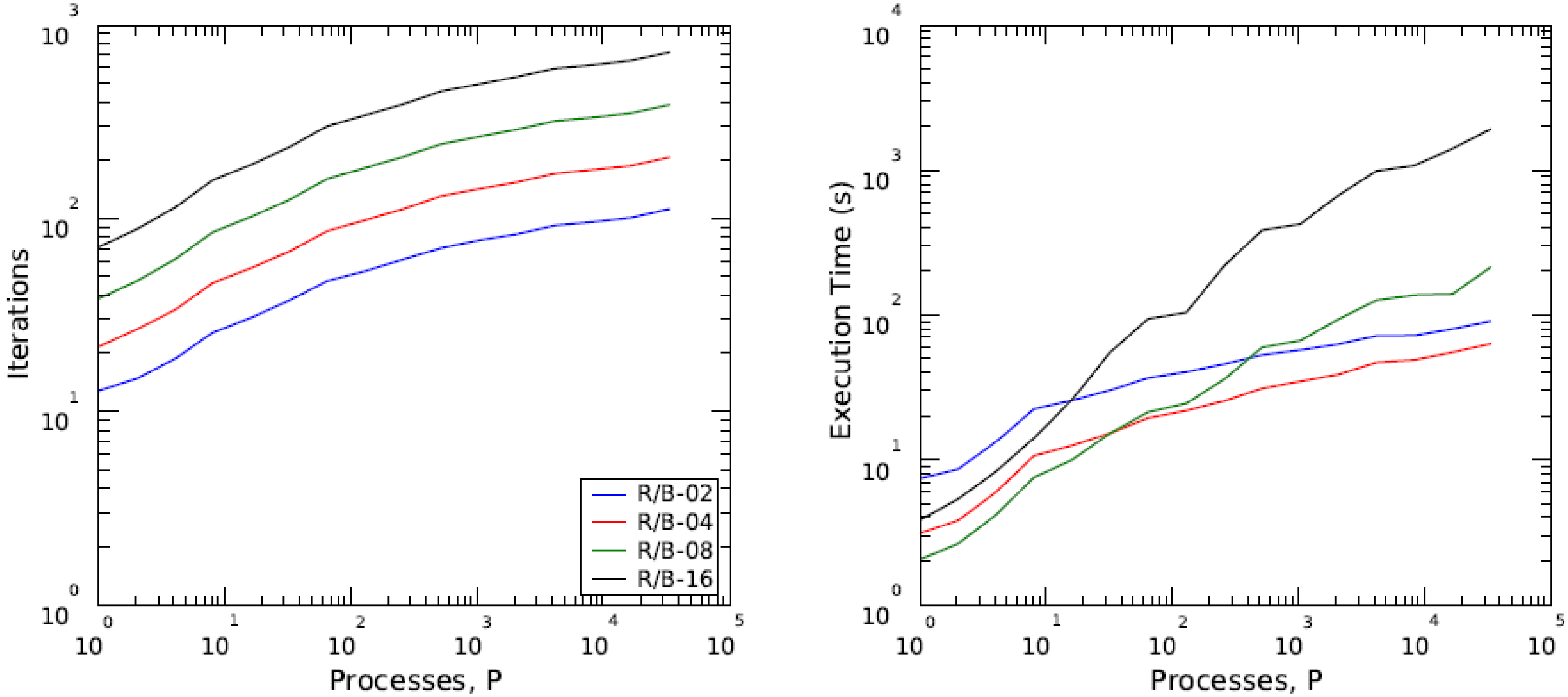
6. Construction *vs* Solution Time

- **Total execution time = construction time + iterative solution time:**
  - Construction time: independent of *c* & *h* ⇨ average over all cases
  - Iterative solution depicted for *c* = 0.9 & *h* = 0.1 cm as example



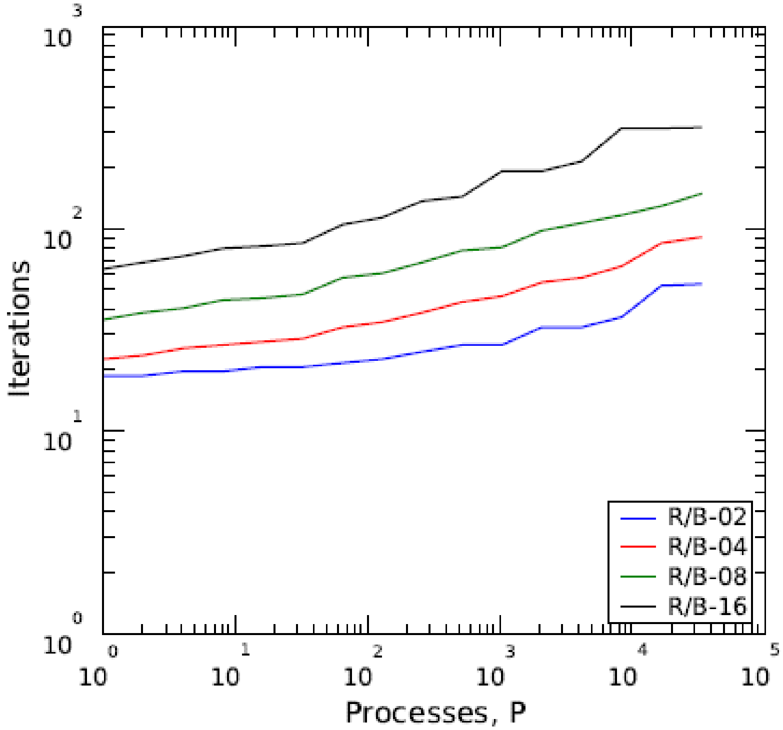
Weak Scaling Results

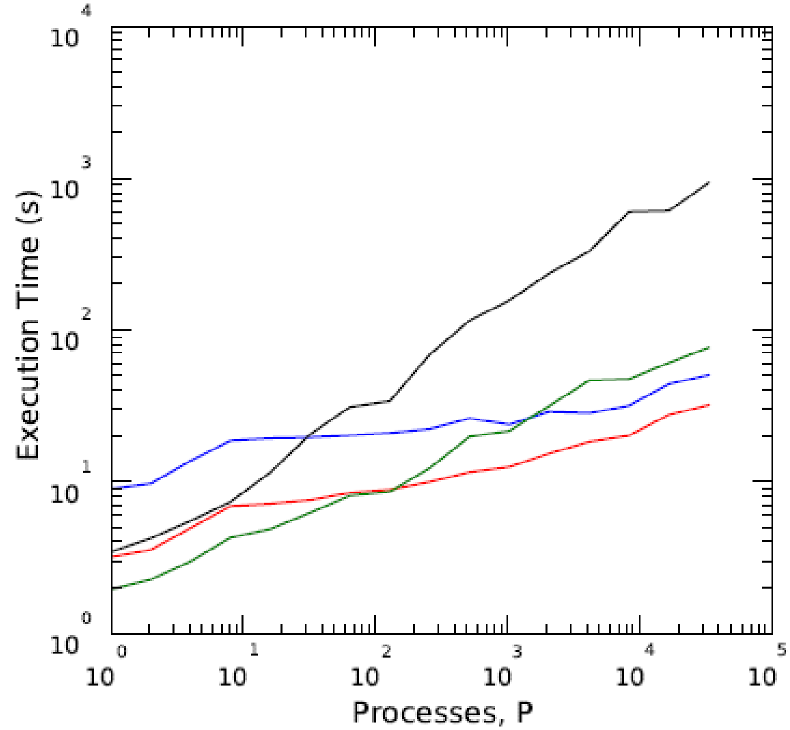
- c=0.9, h=0.1



Weak Scaling Results

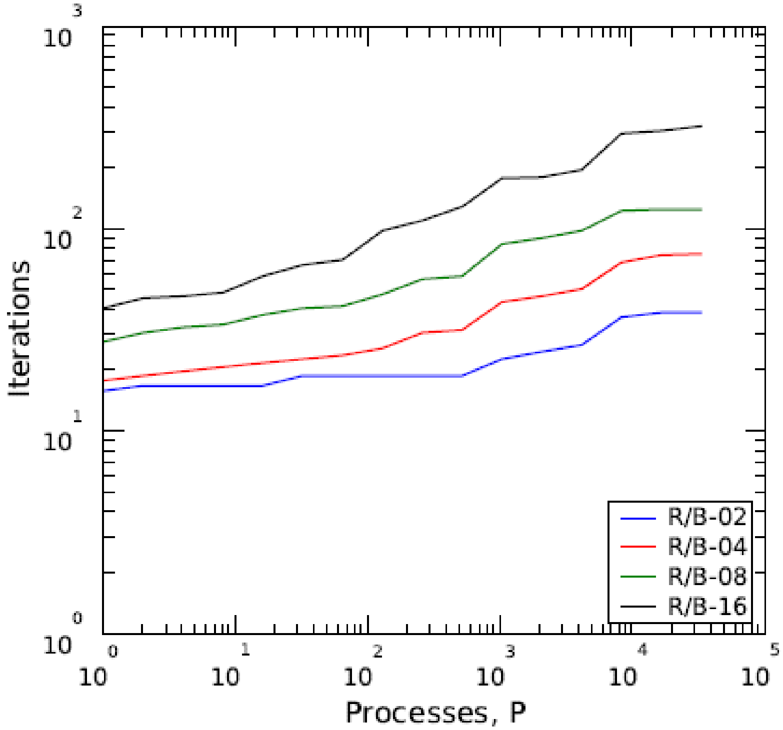
- **c=0.9, h=1.0**

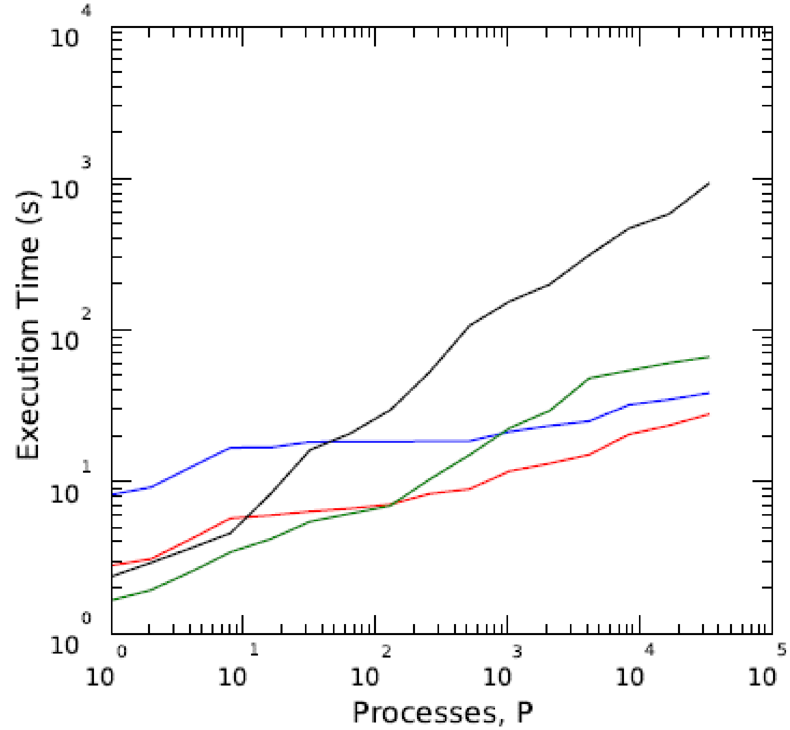




Weak Scaling Results

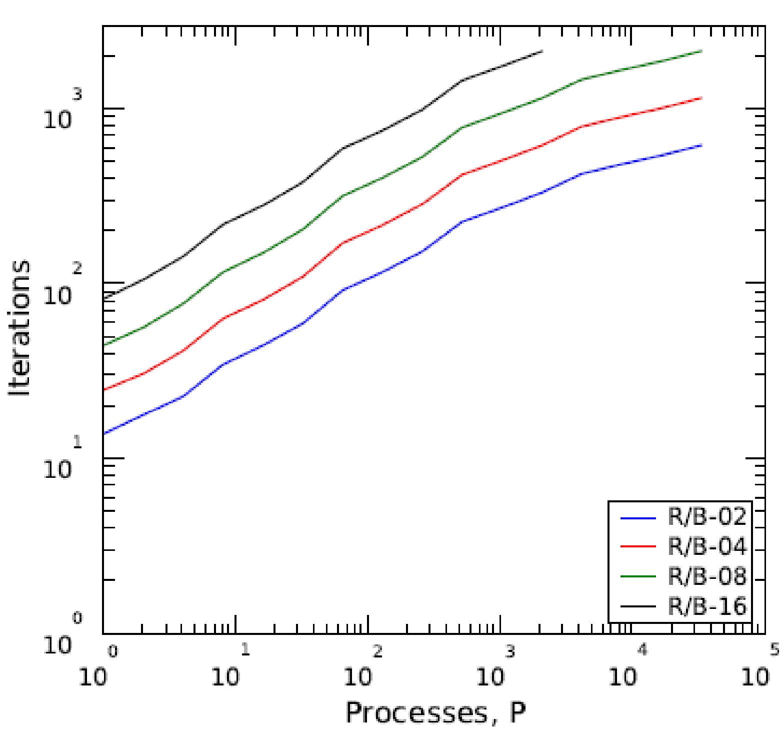
- c=0.9, h=10.0

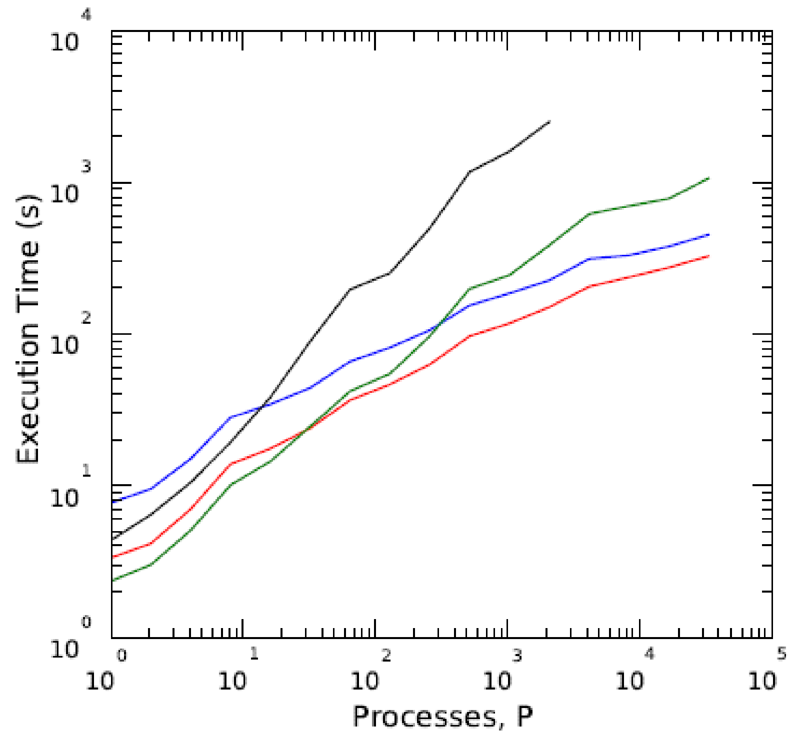




Weak Scaling Results

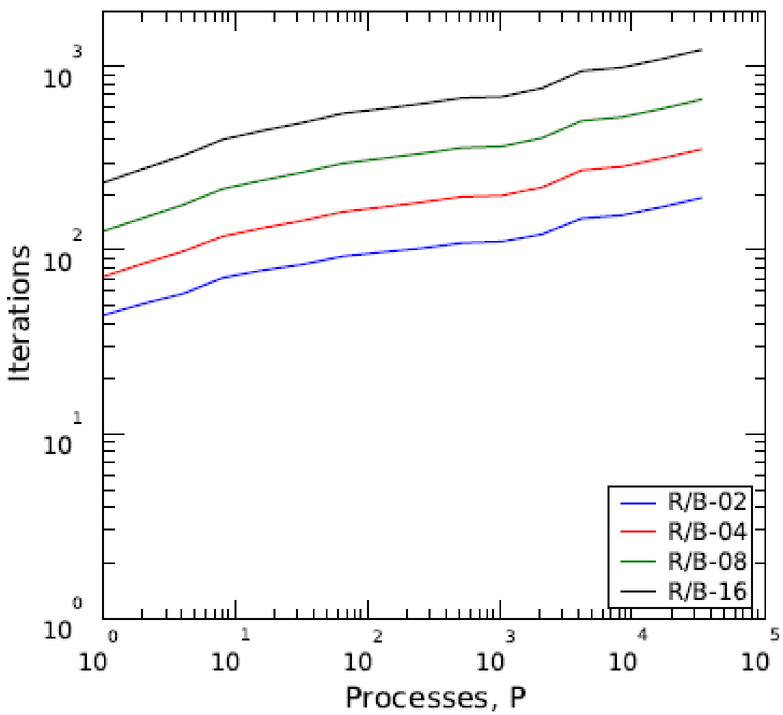
- c=0.99, h=0.1

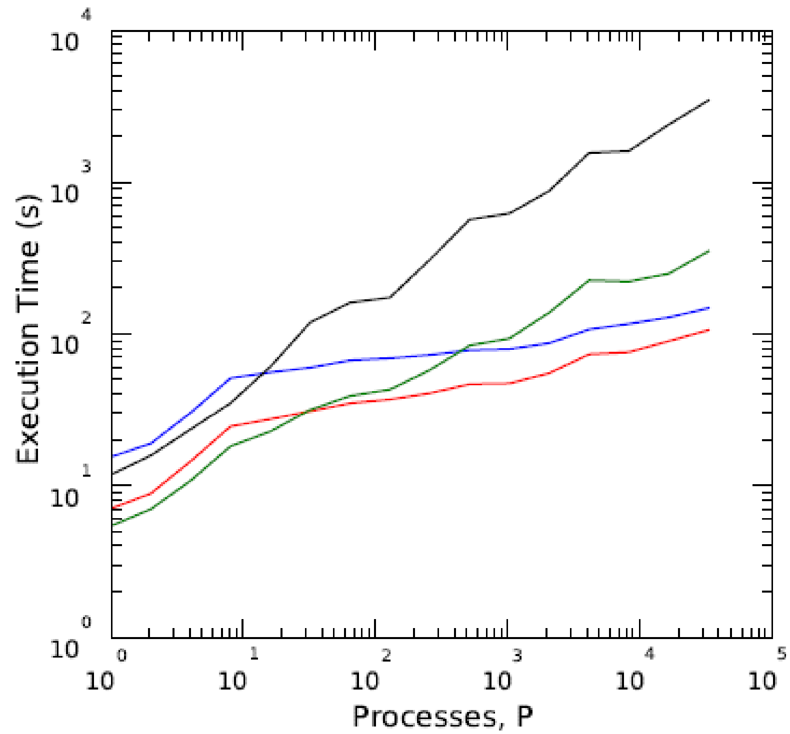




Weak Scaling Results

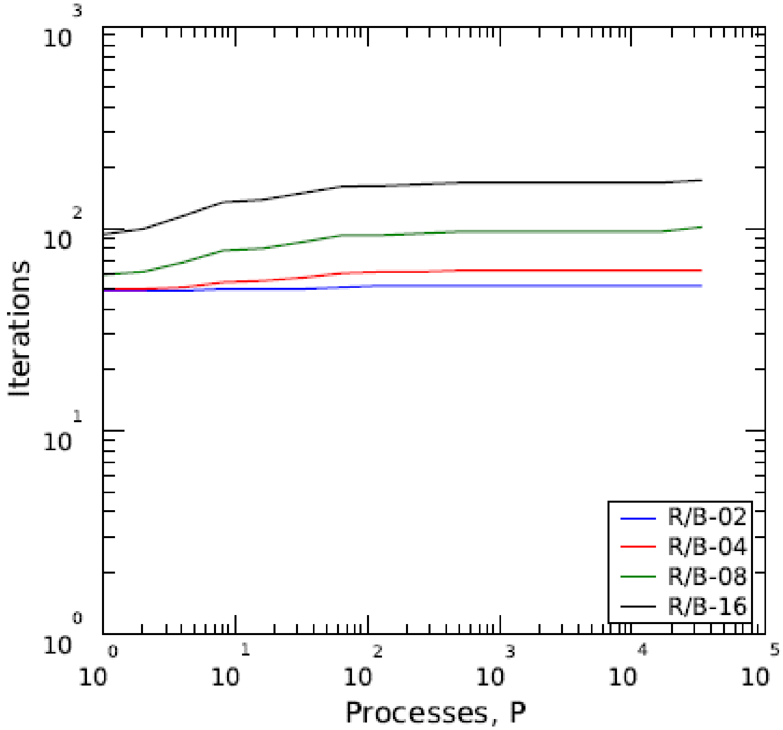
- c=0.99, h=1.0

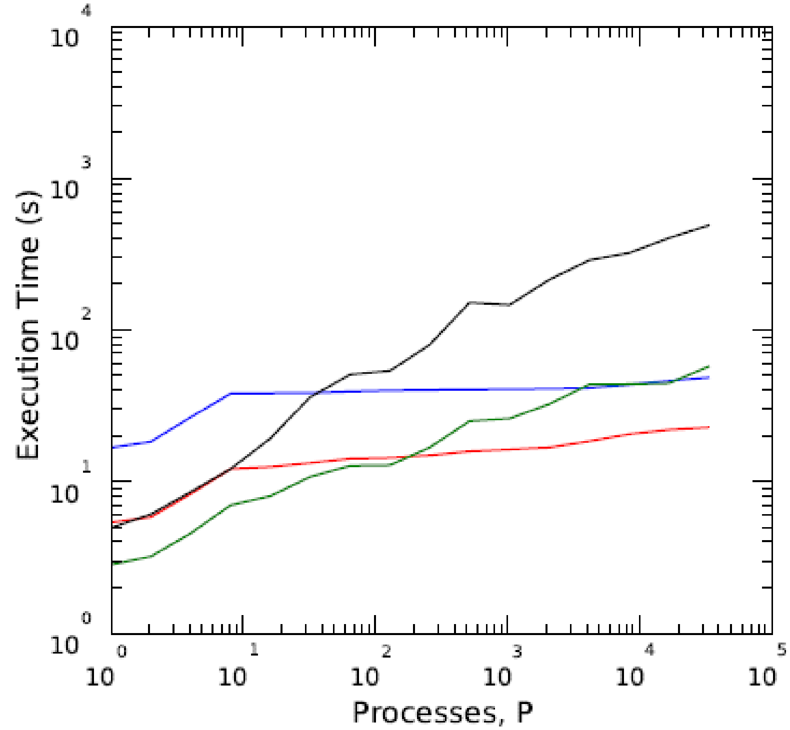




Weak Scaling Results

- c=0.99, h=10.0



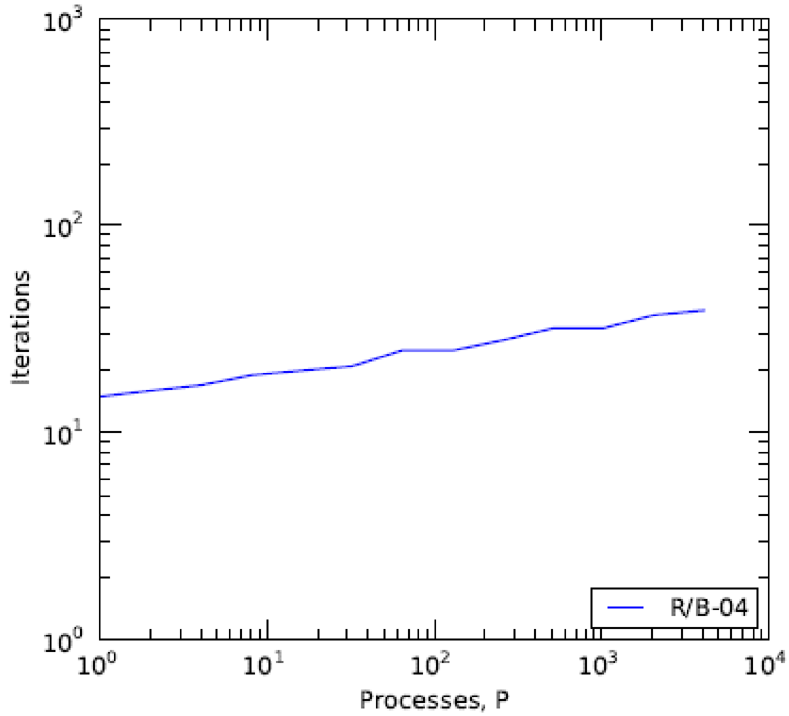


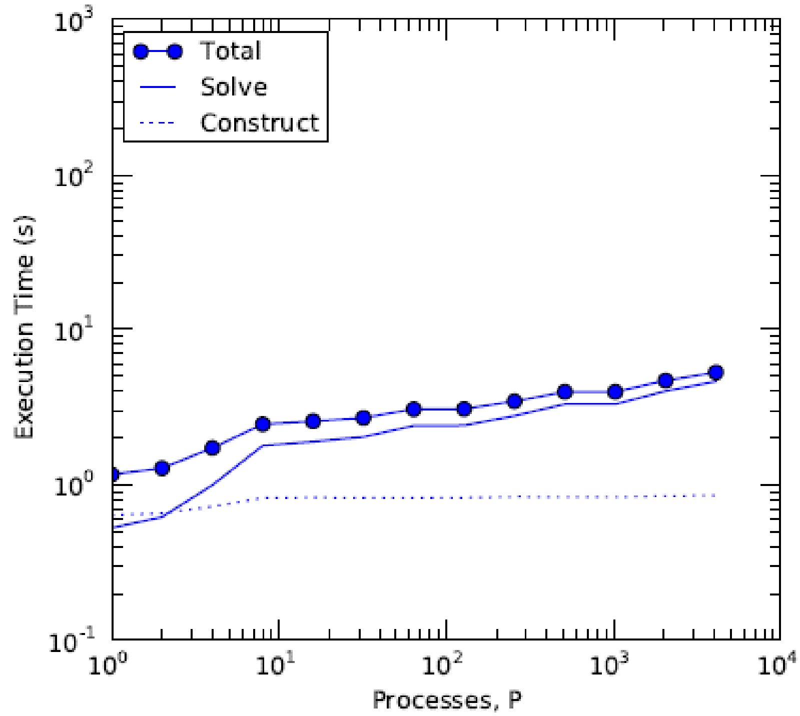
Periodic Heterogeneous Layers

- Alternating layers of optically thin and thick materials
- Known challenge for SI-DSA convergence
- ITMM explicitly couples thick and thin materials
- Starting with h=1, increase every other layer by a factor of ‘a’ and decrease the other layers by a factor of ‘a’

PHL Weak Scaling Results

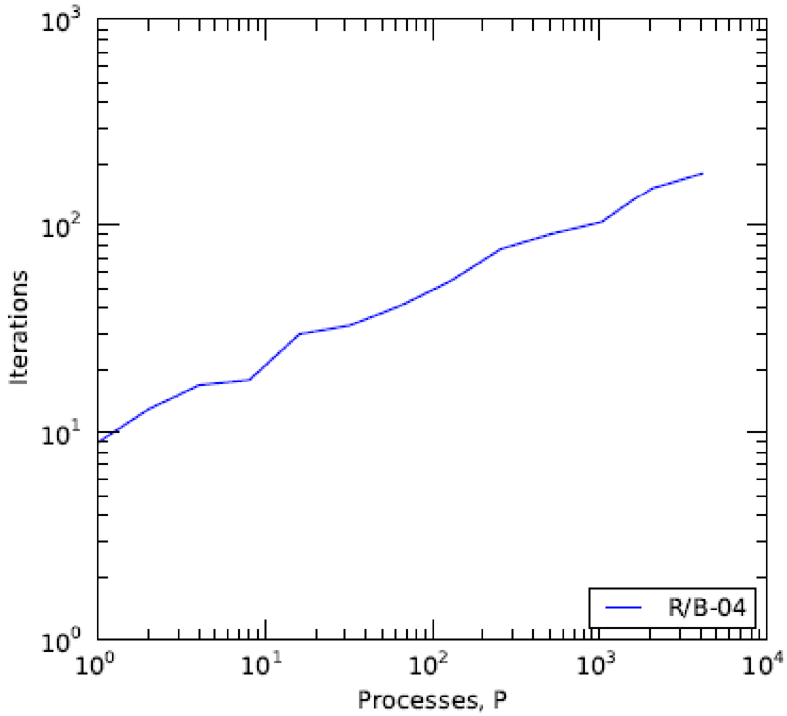
- c=0.9, a=10

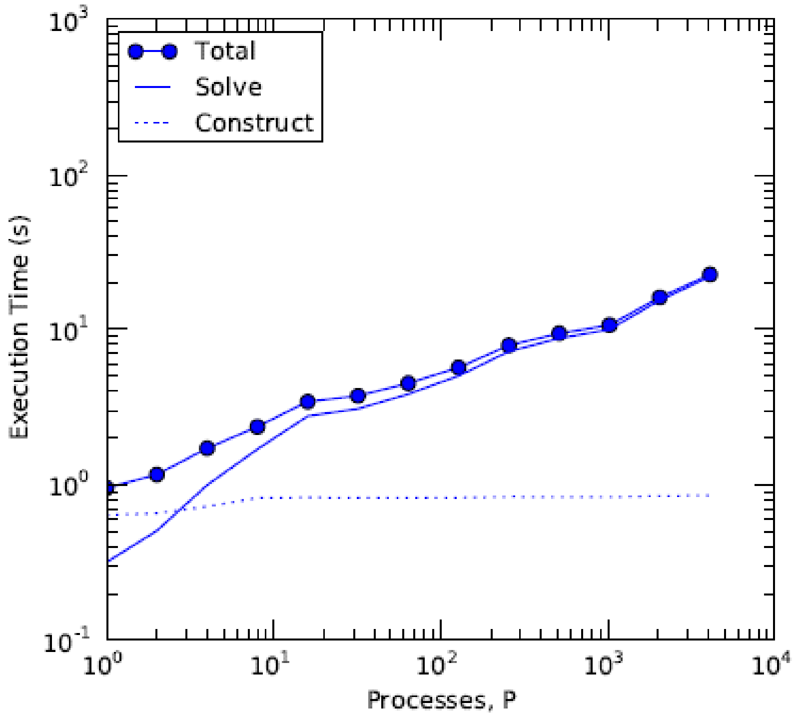




PHL Weak Scaling Results

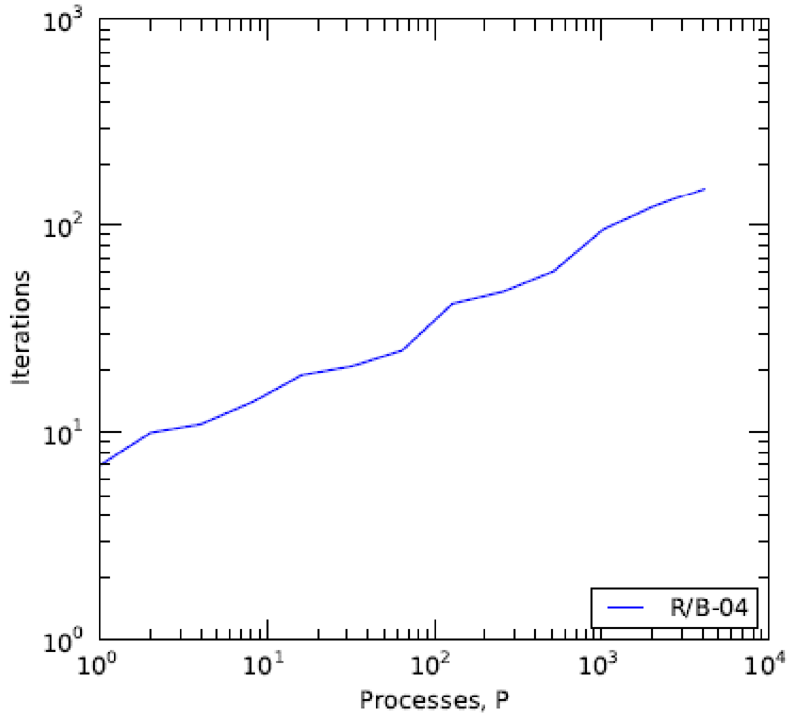
- c=0.9, a=100

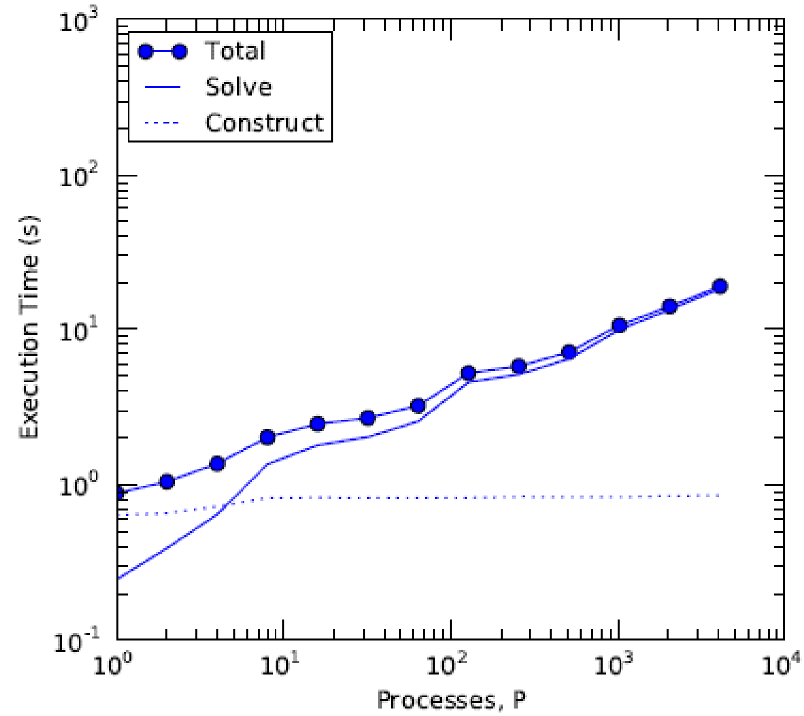




PHL Weak Scaling Results

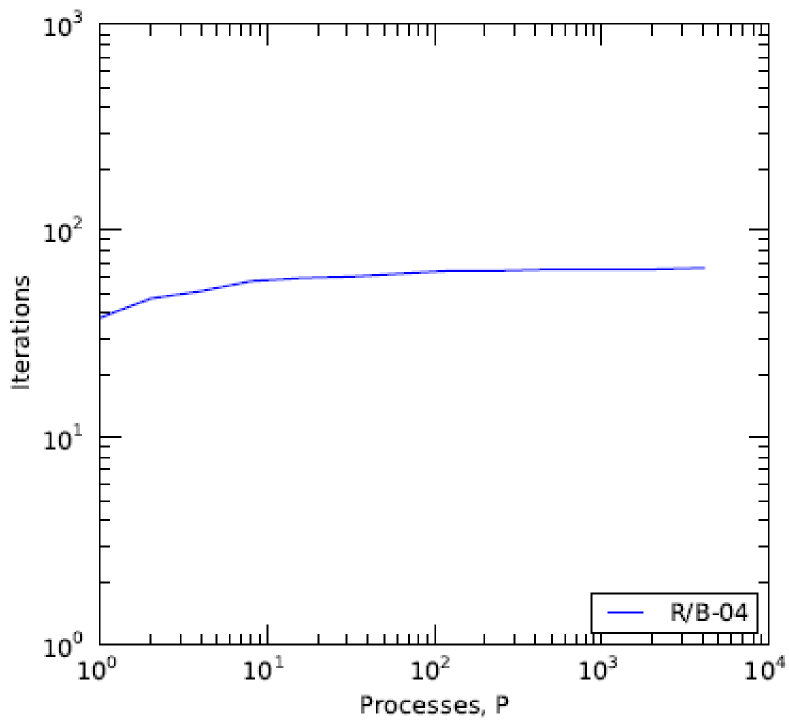
- c=0.9, a=1000

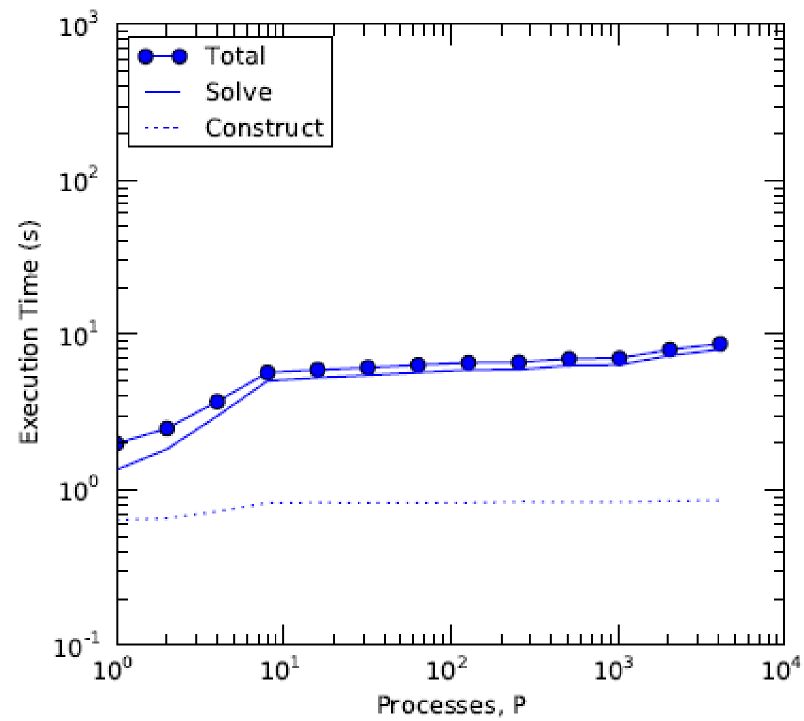




PHL Weak Scaling Results

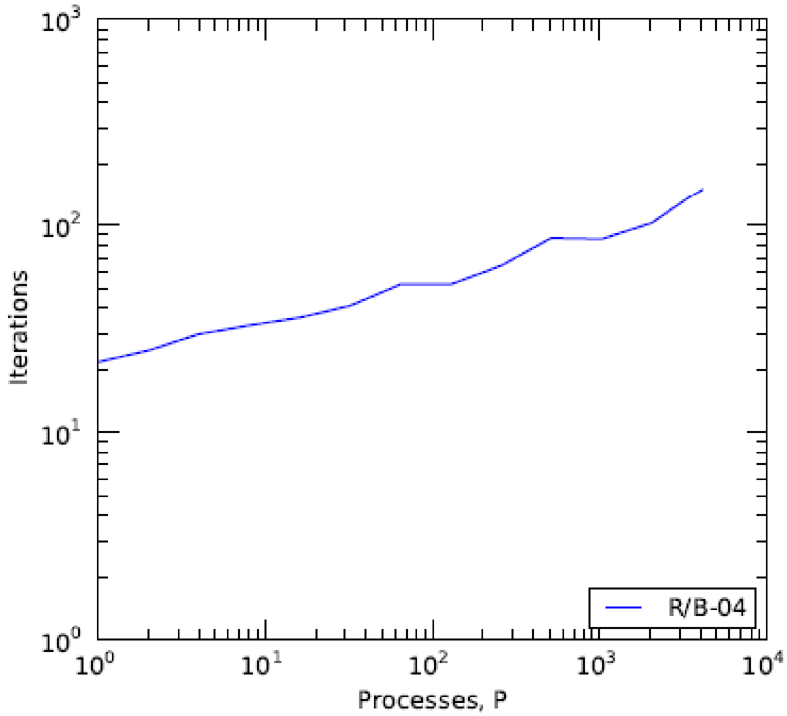
- c=0.99, a=10

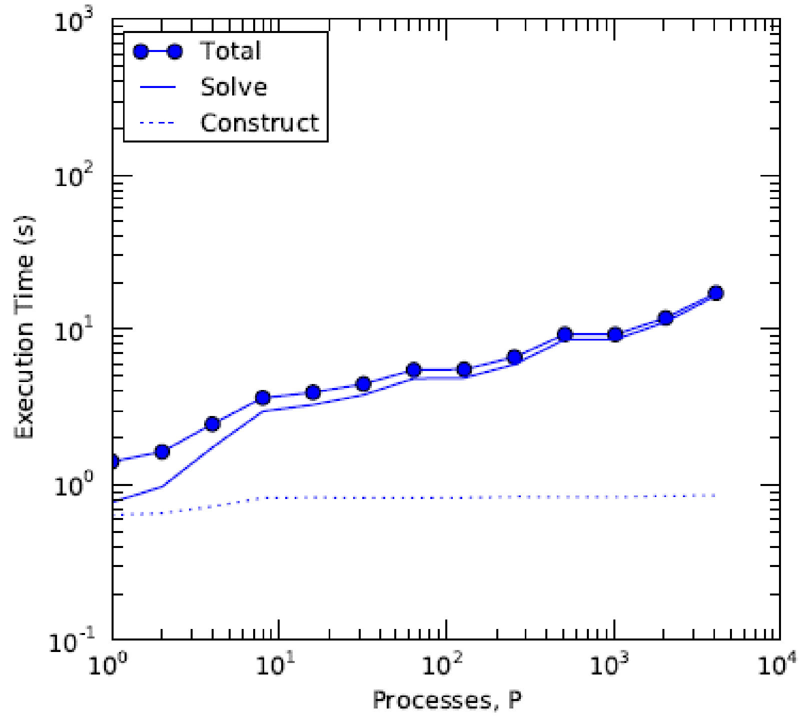




PHL Weak Scaling Results

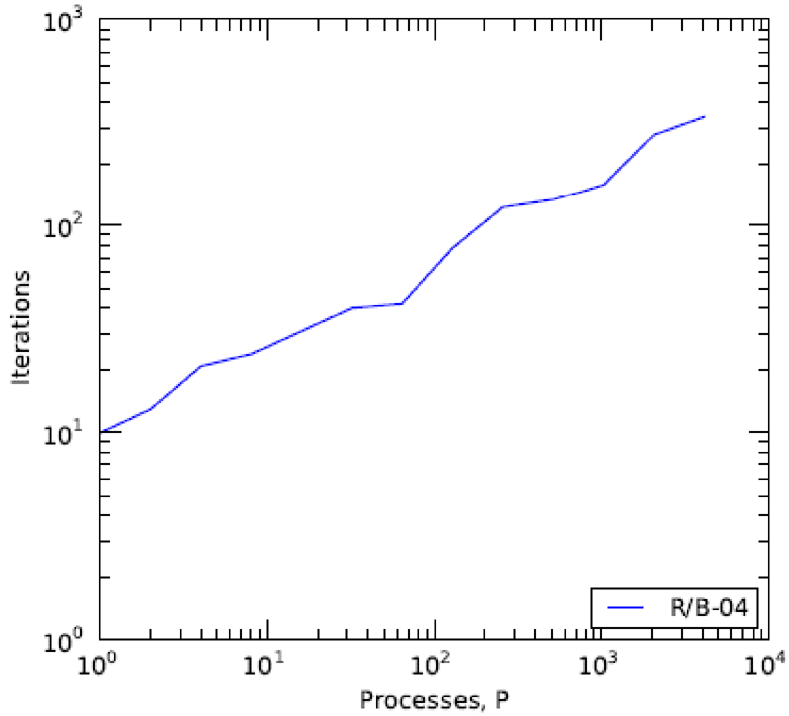
- c=0.99, a=100

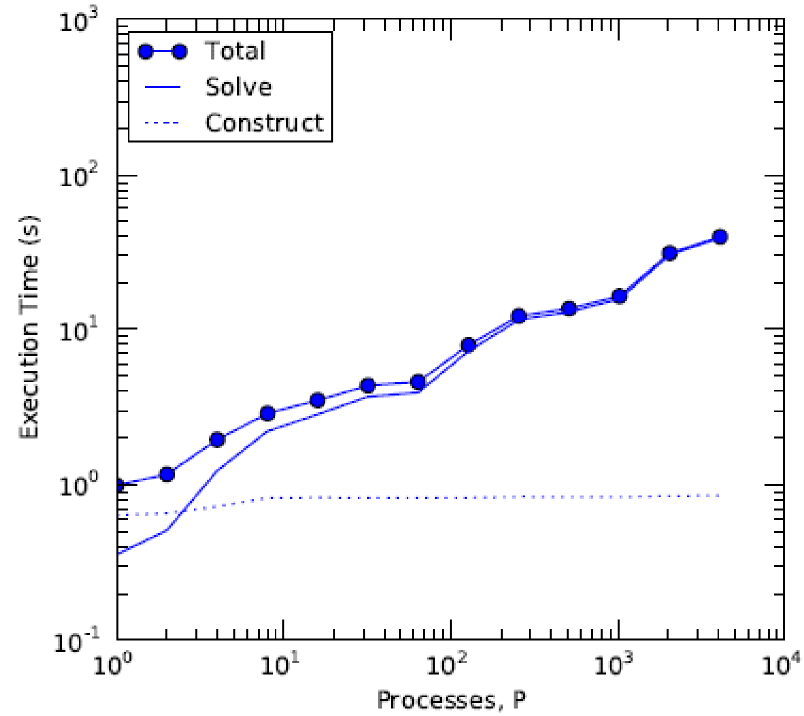




PHL Weak Scaling Results

- c=0.99, a=1000





7. Conclusions

7. Conclusions

- **The Nuclear Computational Science Group at NC State is engaged in broad span of topics**
- **Topic illustrated today: Multiprocessing strategies particularly suited for massively parallel architectures**
  - ITMM SDD avoids sequential mesh-sweeps
  - Considered BJ & GS parallelizations: PGS bests PBJ
  - Compared PGS to traditional KBS in PARTISN:
    - Very large differences when SI is accelerated with DSA
    - Gap closes as optical thickness and scattering ratio are increased ⇨ most difficult SI problems
    - SI & SI-DSA demonstrate larger growth in execution time as *P* ↑
    - Conclusions must be validated for *P* > 1,024
- **PGS performance should improve with suitable preconditioner: difficult**