A New Method for Computation of Self-gravity in an Isolated System

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Outline

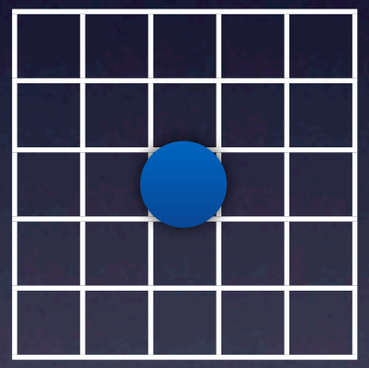
- Problem with Fast Fourier Transform
- Methods:
  1) Green's function
  2) Multipole correction
- Comparison
- Conclusion

Fast Fourier Transform (FFT)

Poisson Equation:

$$\nabla^2 \phi(\mathbf{x}) = \rho(\mathbf{x})$$

$$\hat{\phi}(\mathbf{k}) = -\frac{\hat{\rho}(\mathbf{k})}{k^2}$$



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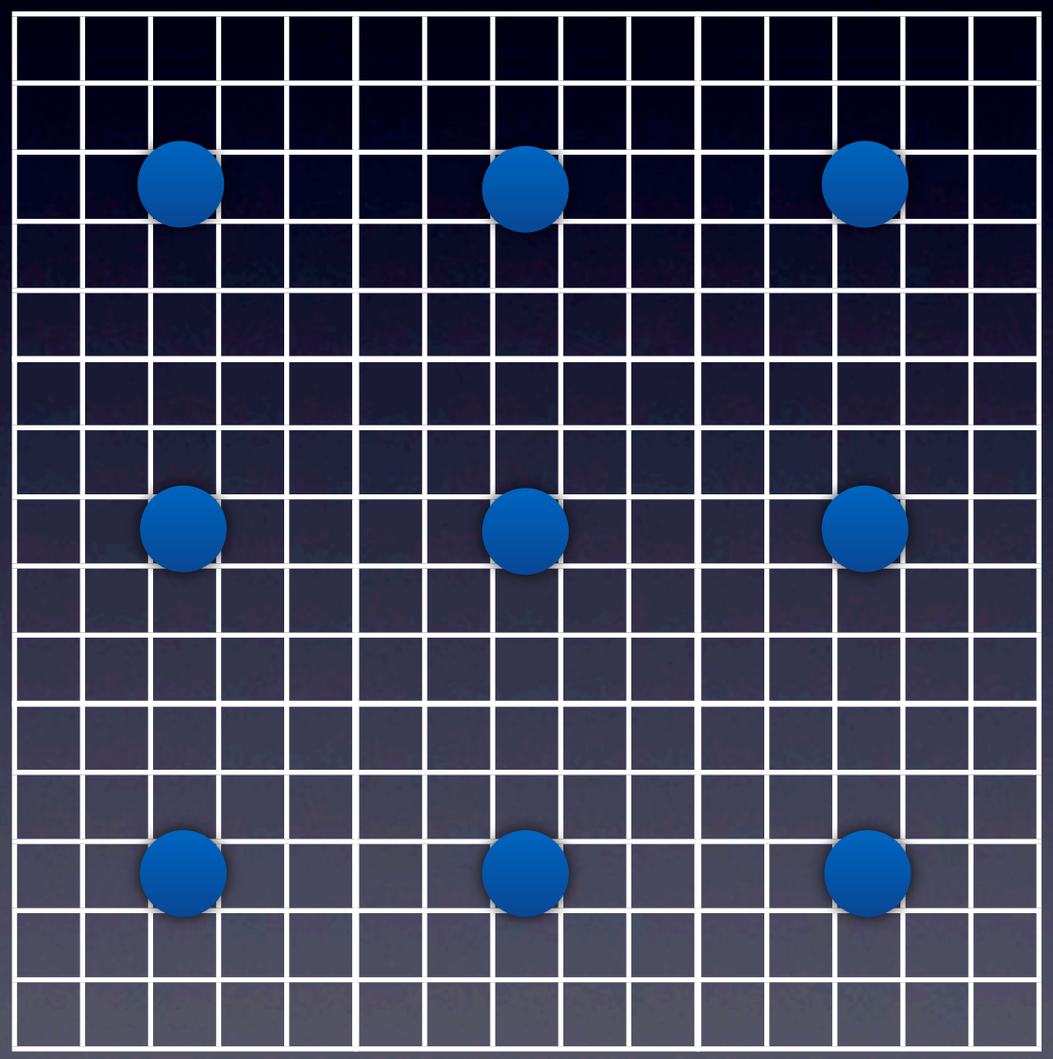
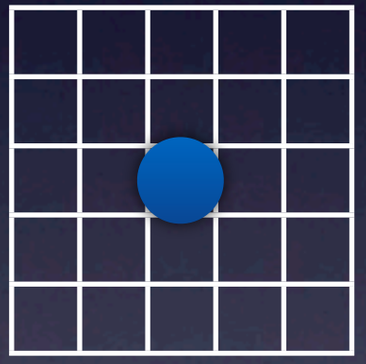


Periodic Boundary Condition

Zero Padding



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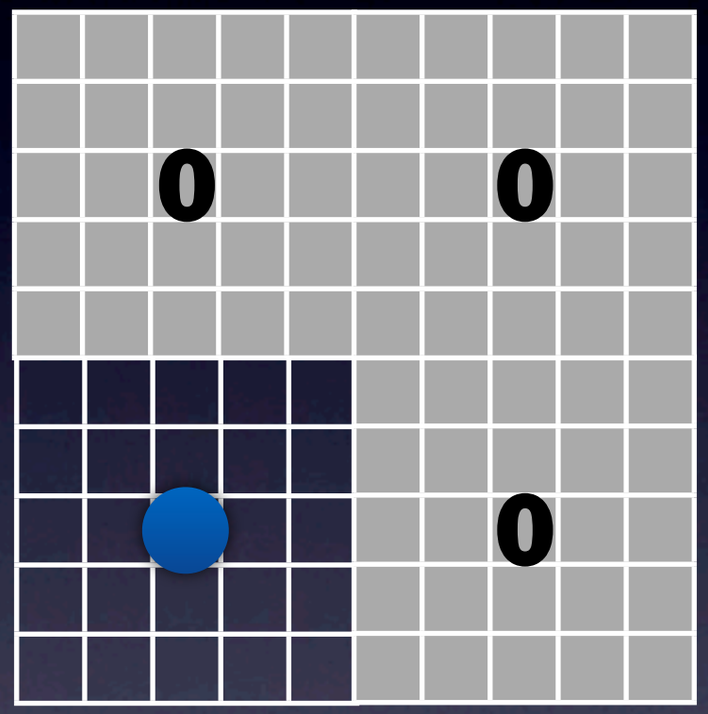
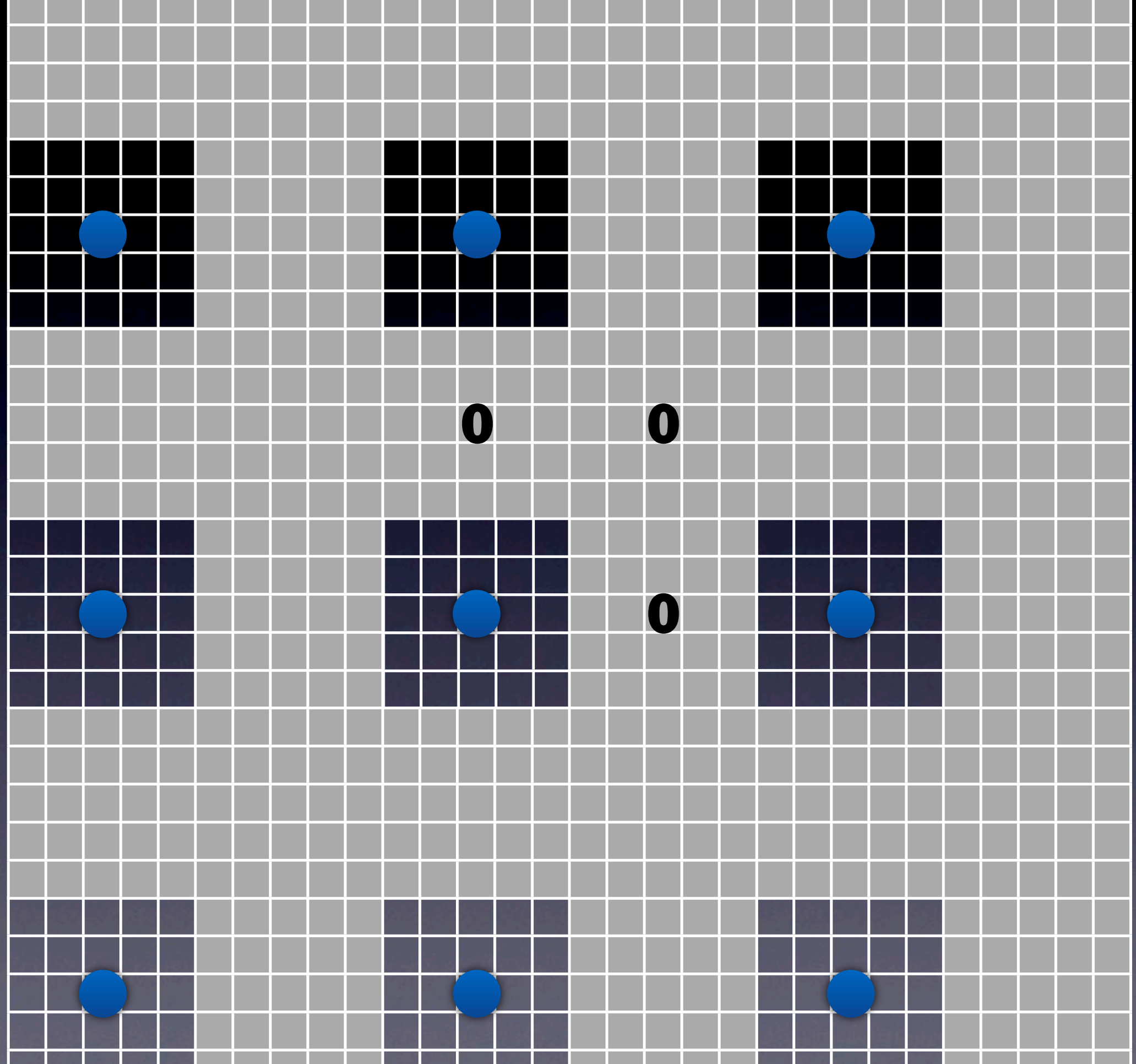



0
0
0

Green's Function

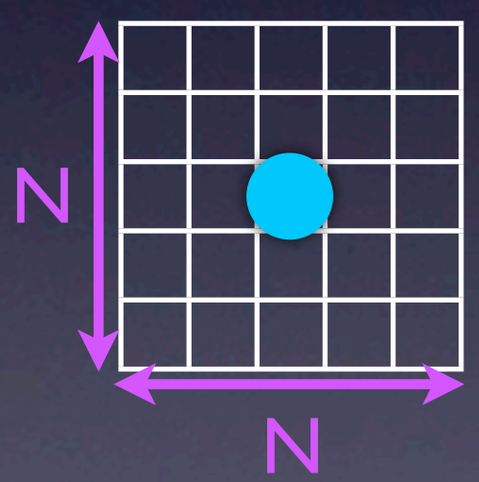
$$G(\mathbf{x}) = -\frac{1}{4\pi|\mathbf{x}|}$$

$$\nabla^2 G(\mathbf{x}) = \delta(\mathbf{x})$$

$$\phi(\mathbf{x}) = \int G(\mathbf{x}-\mathbf{x}')\rho(\mathbf{x}')d^3x'$$

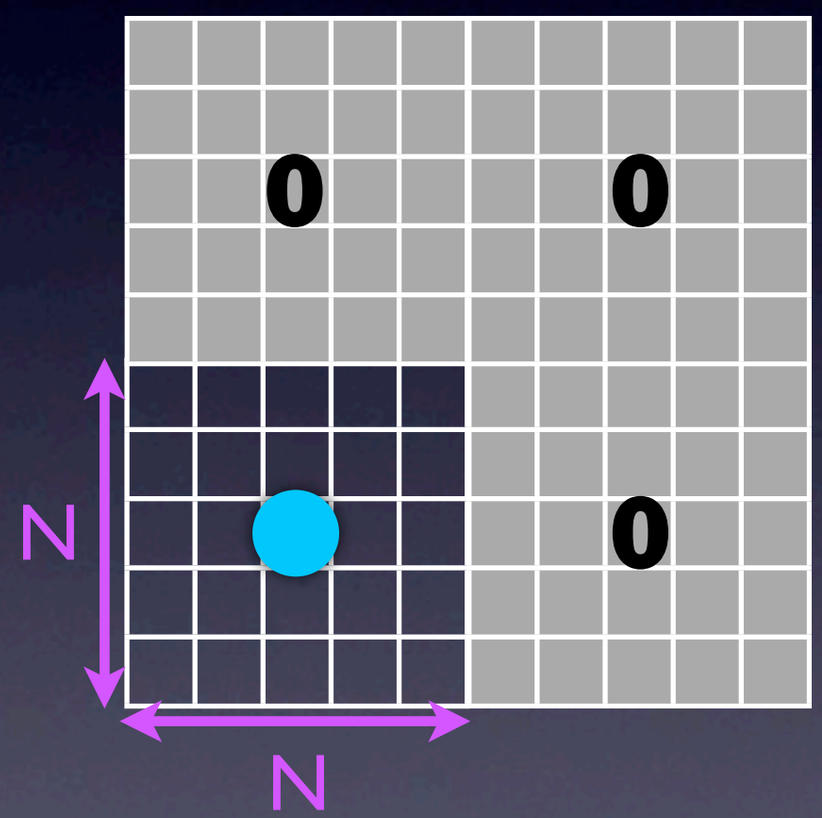
$$\hat{\phi}(\mathbf{k}) = \hat{G}(\mathbf{k})\hat{\rho}(\mathbf{k})$$

Green's Function



(Budiardja et. al. 2011)

Green's Function



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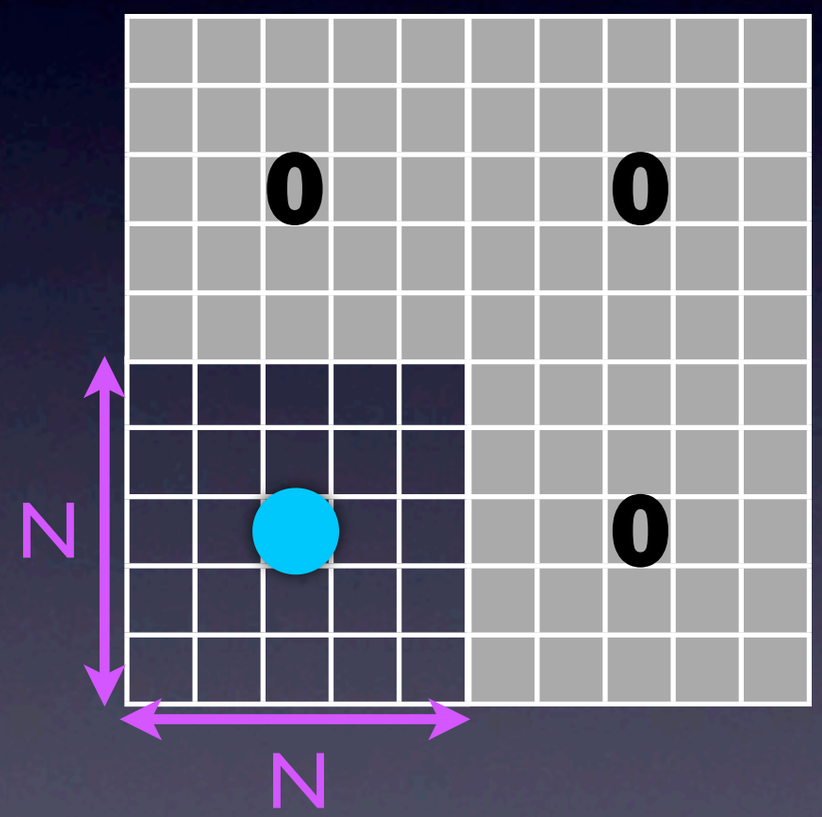
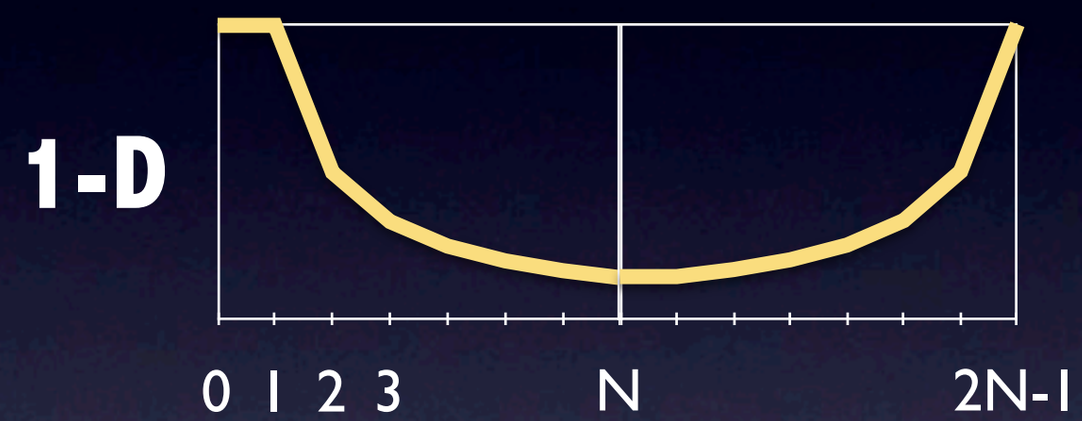
Green's Function



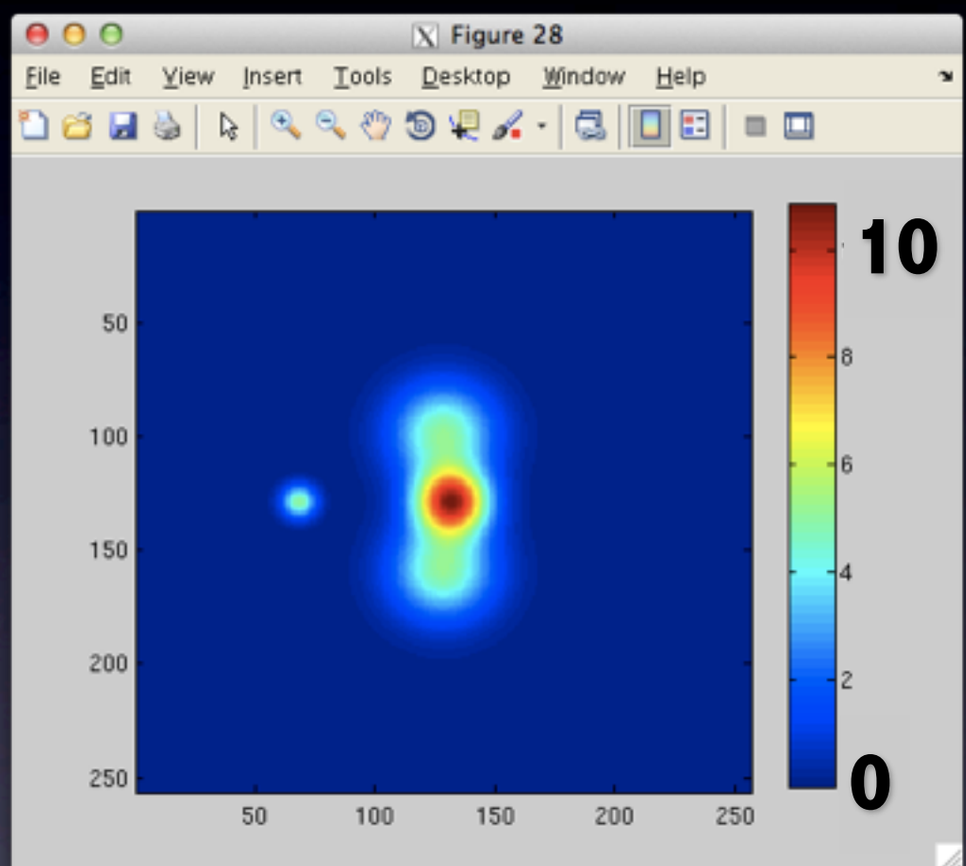


$$G_i = -\frac{1}{4\pi\sqrt{i}} = G_{2N-i} \qquad 1 \le i \le N$$

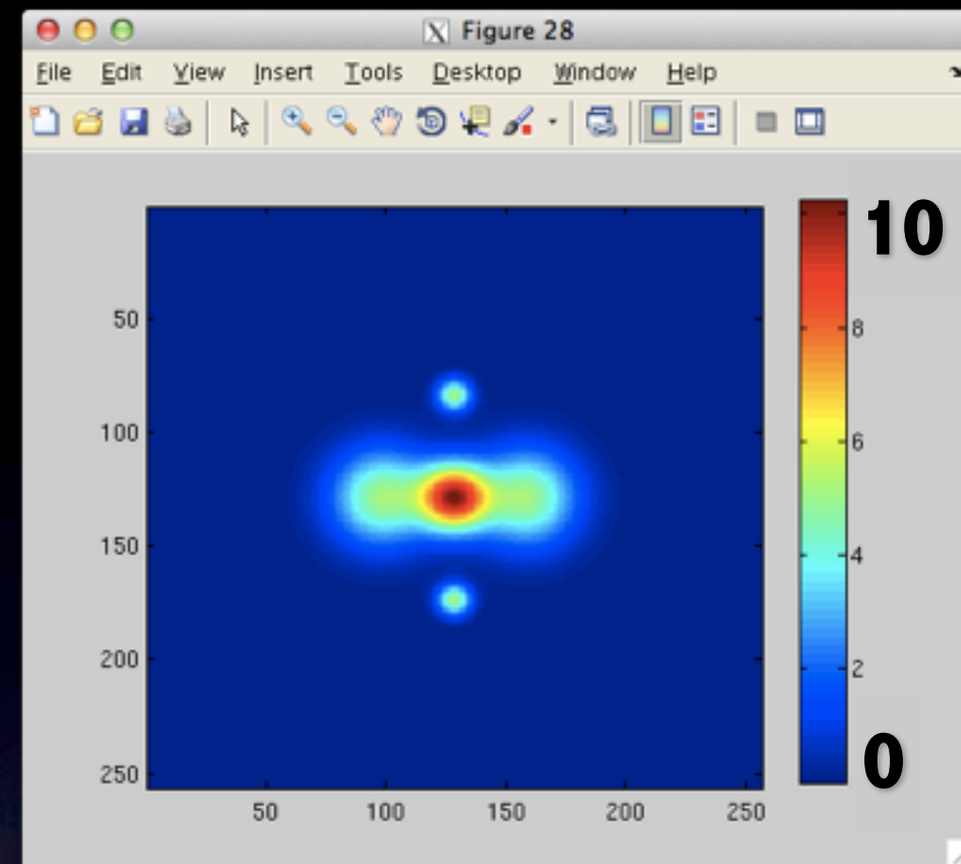
$$G_0 = -\frac{1}{4\pi}$$

(Budiardja et. al. 2011)

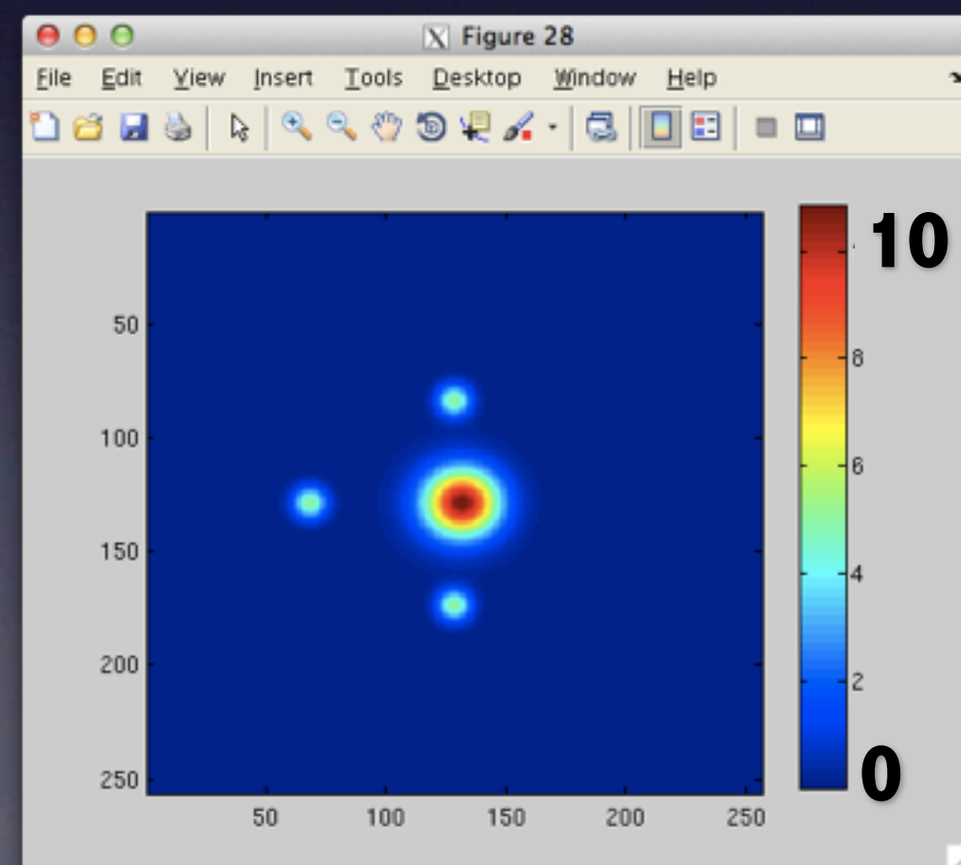
Density



x=0

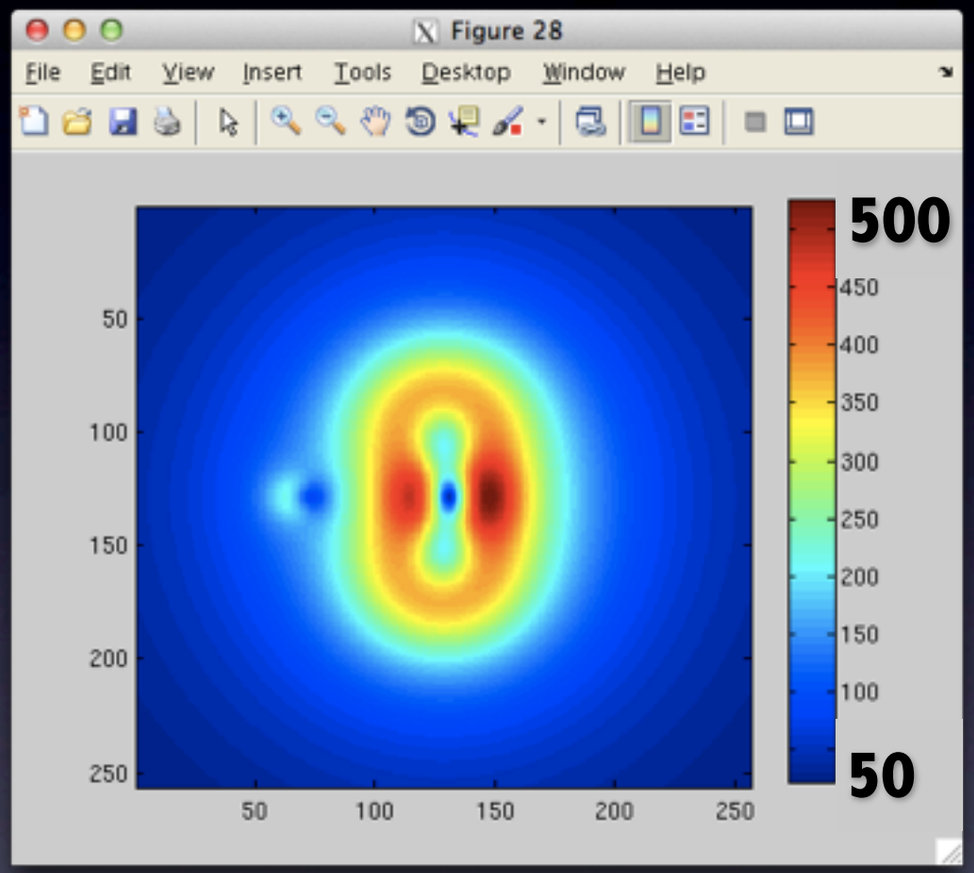


y=0

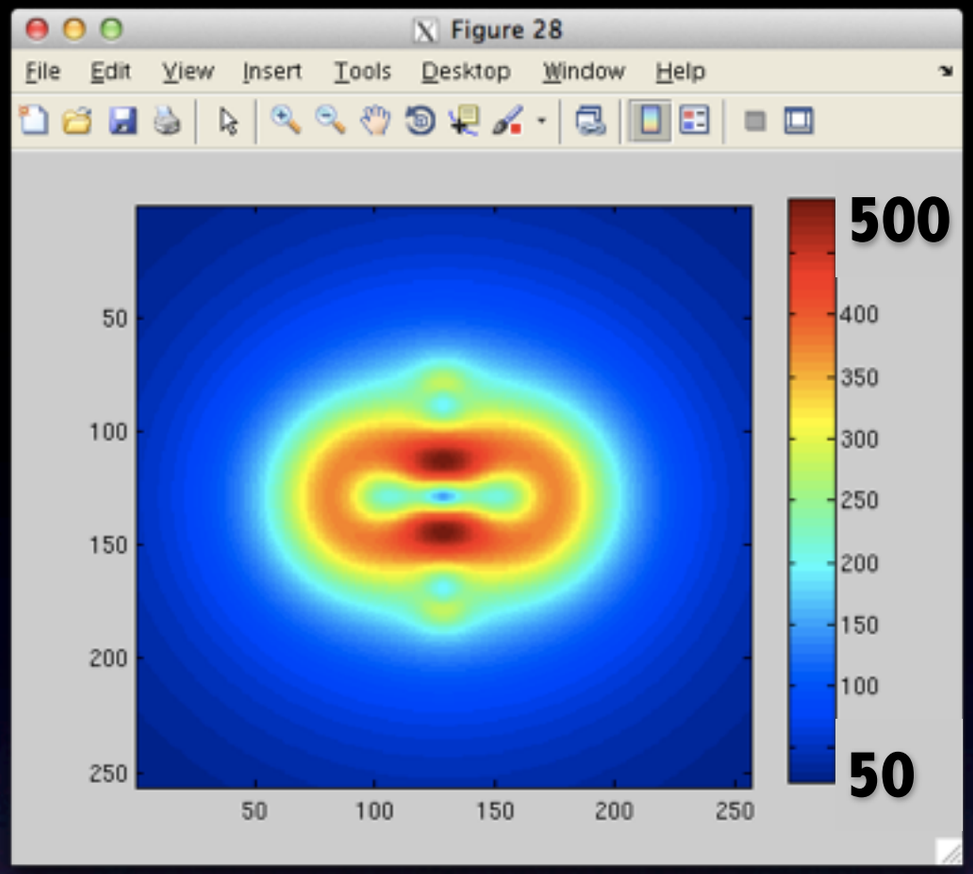


z=0

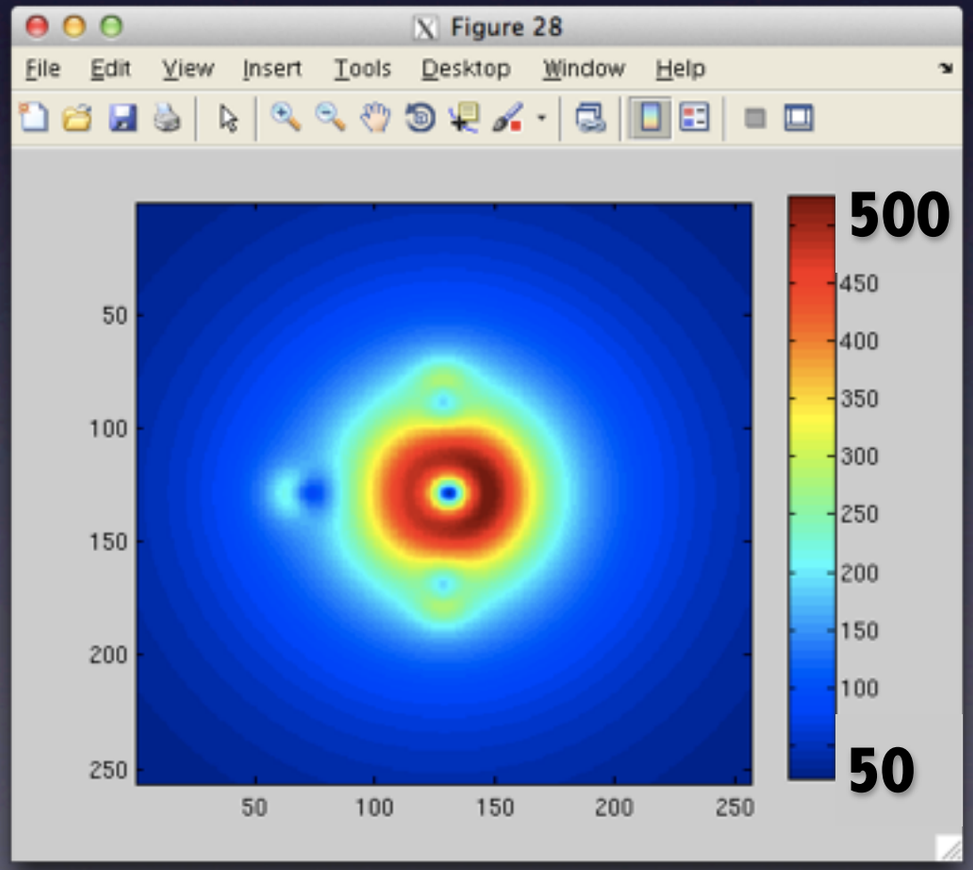
Force: $\left|\mathbf{F}_{\text{analy}}\right|$



x=0



y=0

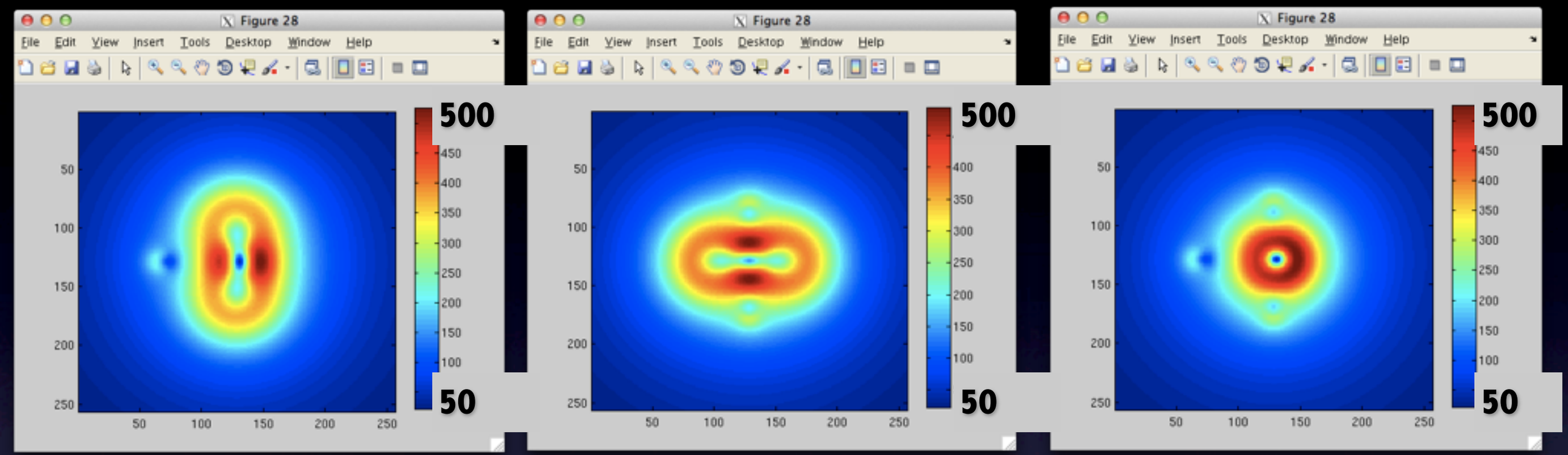


z=0

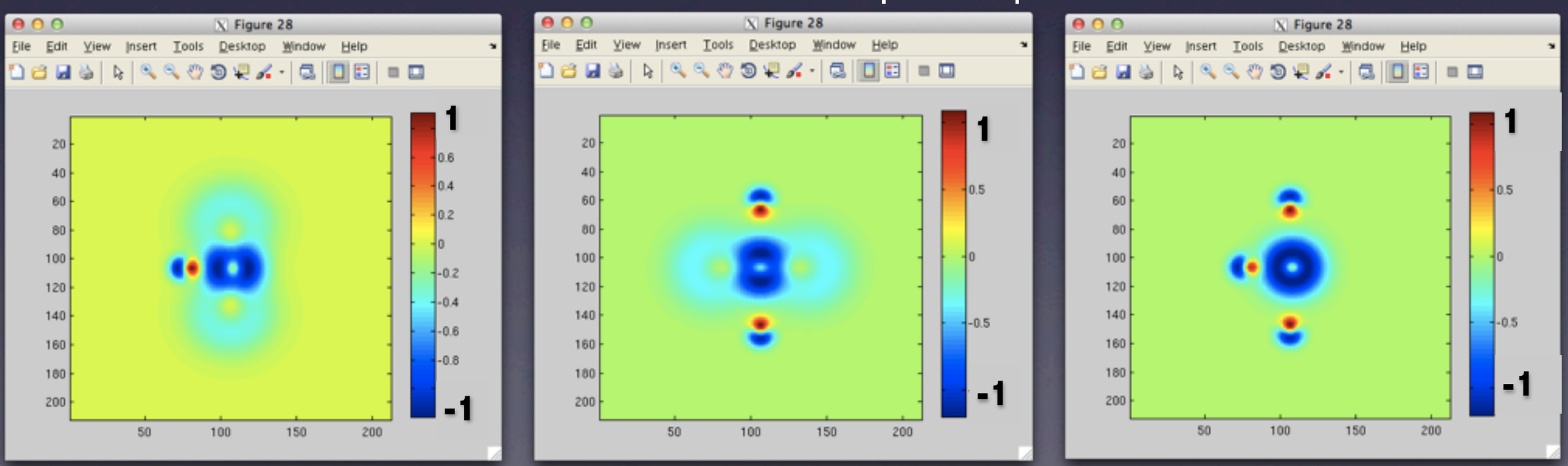
Procedure

- Potential from FFT with Green's function method
- Force from finite difference method with fourth-order accuracy
- Error is defined as, $\varepsilon_{\mathrm{FFT}} = \left|\mathbf{F}_{\mathrm{FFT}}\right| - \left|\mathbf{F}_{\mathrm{analy}}\right|$

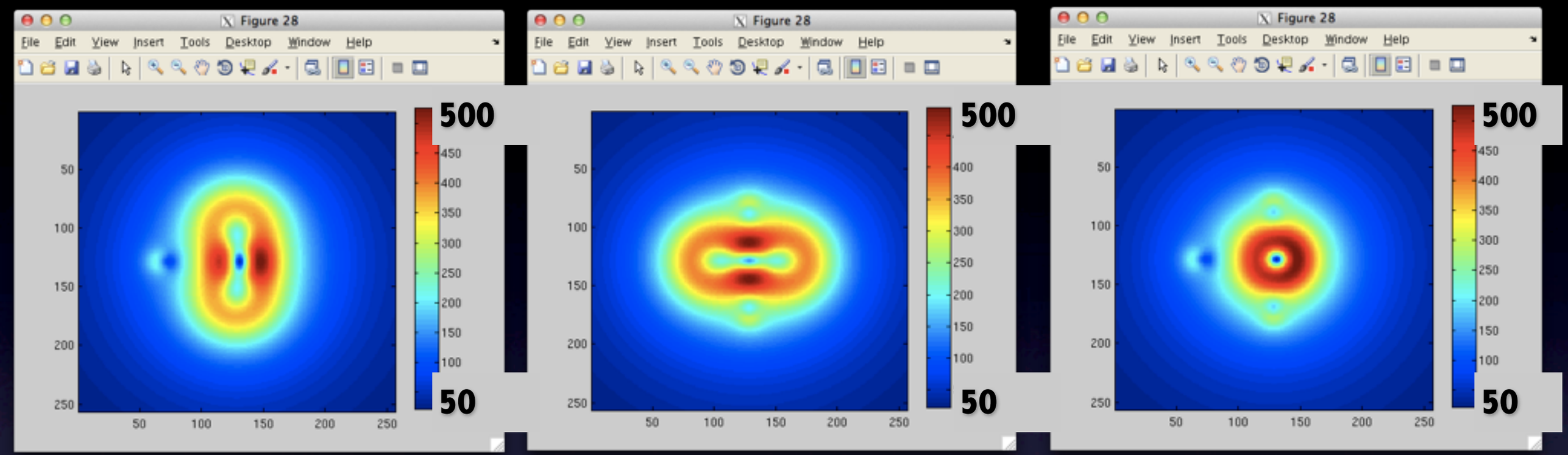
$$\left|\mathbf{F}_{\text{analy}}\right|$$



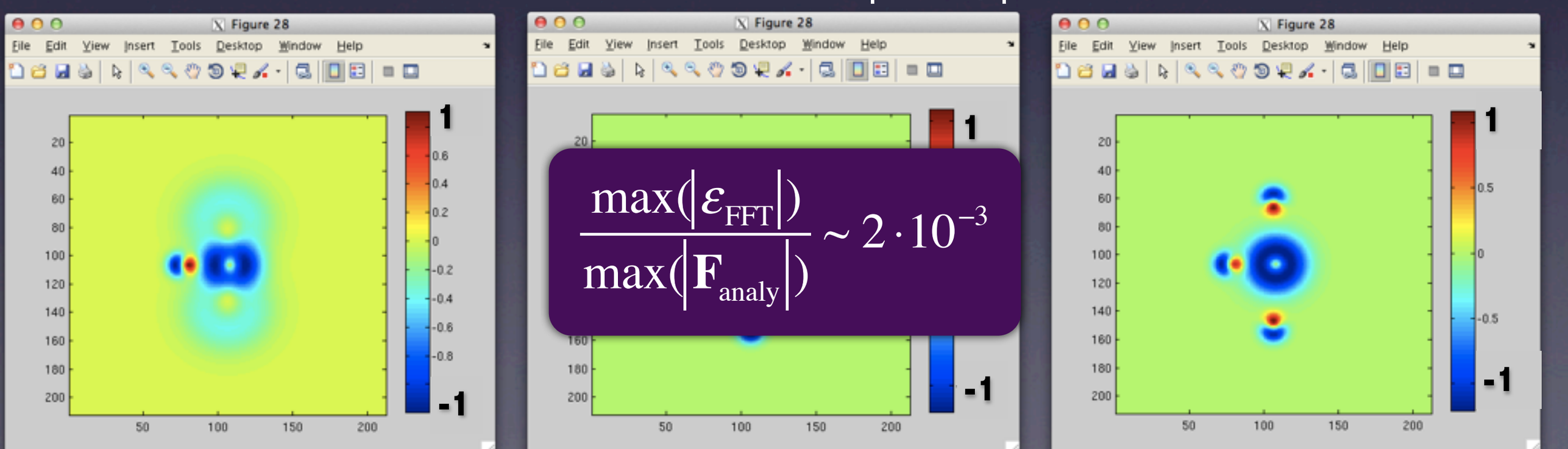
$$\varepsilon_{\text{FFT}} = \left|\mathbf{F}_{\text{FFT}}\right| - \left|\mathbf{F}_{\text{analy}}\right|$$



$$\left|\mathbf{F}_{\text{analy}}\right|$$



$$\varepsilon_{\text{FFT}} = \left|\mathbf{F}_{\text{FFT}}\right| - \left|\mathbf{F}_{\text{analy}}\right|$$

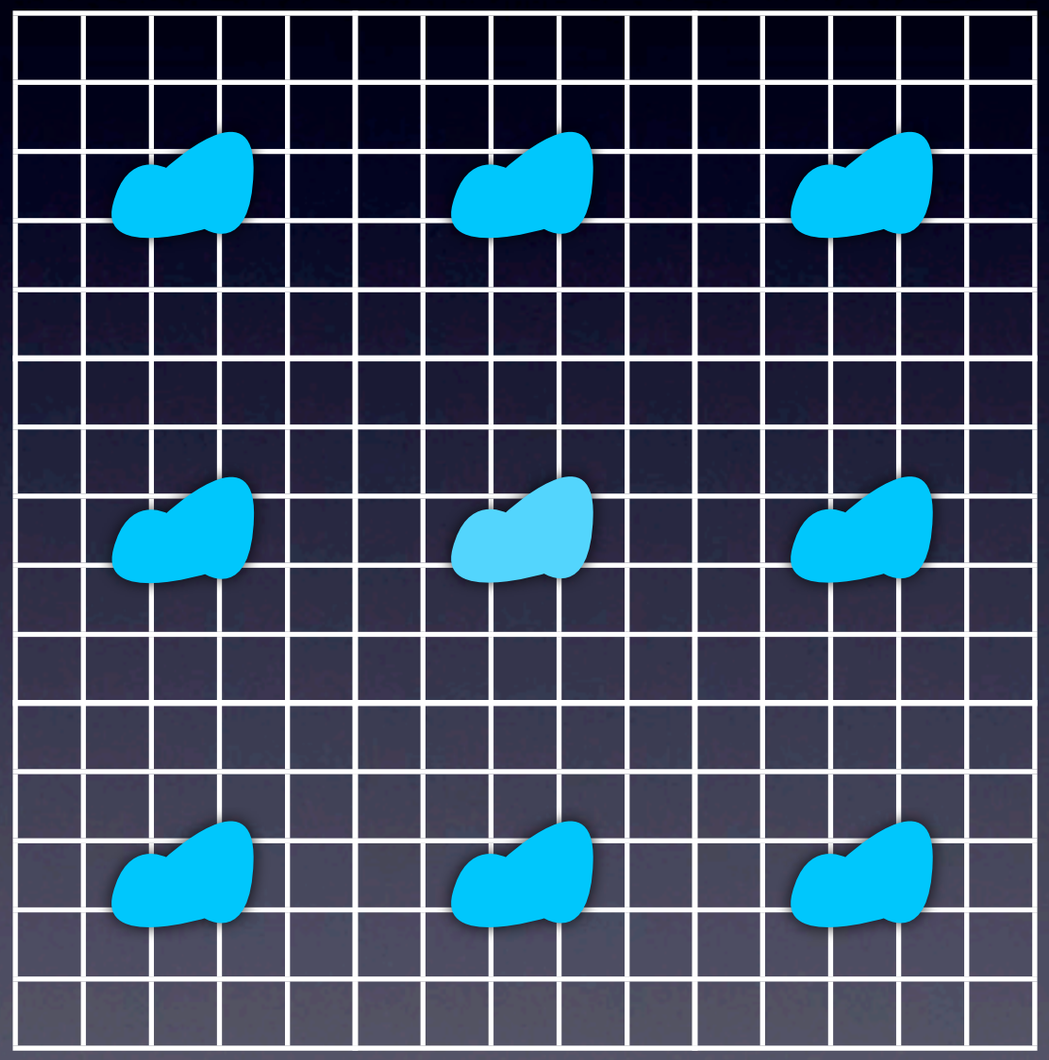


$$\frac{\max(|\varepsilon_{\text{FFT}}|)}{\max(|\mathbf{F}_{\text{analy}}|)} \sim 2 \cdot 10^{-3}$$

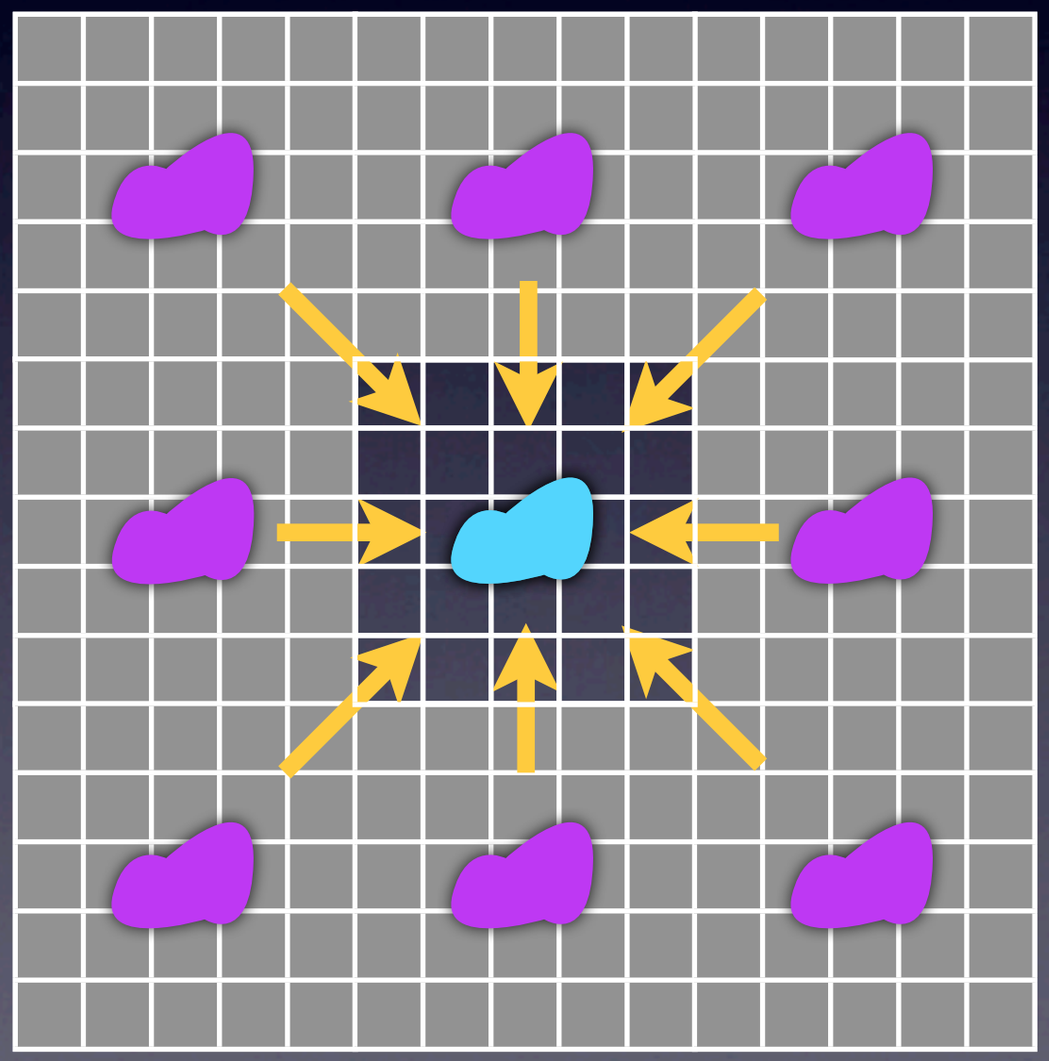
New Method:
Multipole correction

Multipole correction

Multipole correction

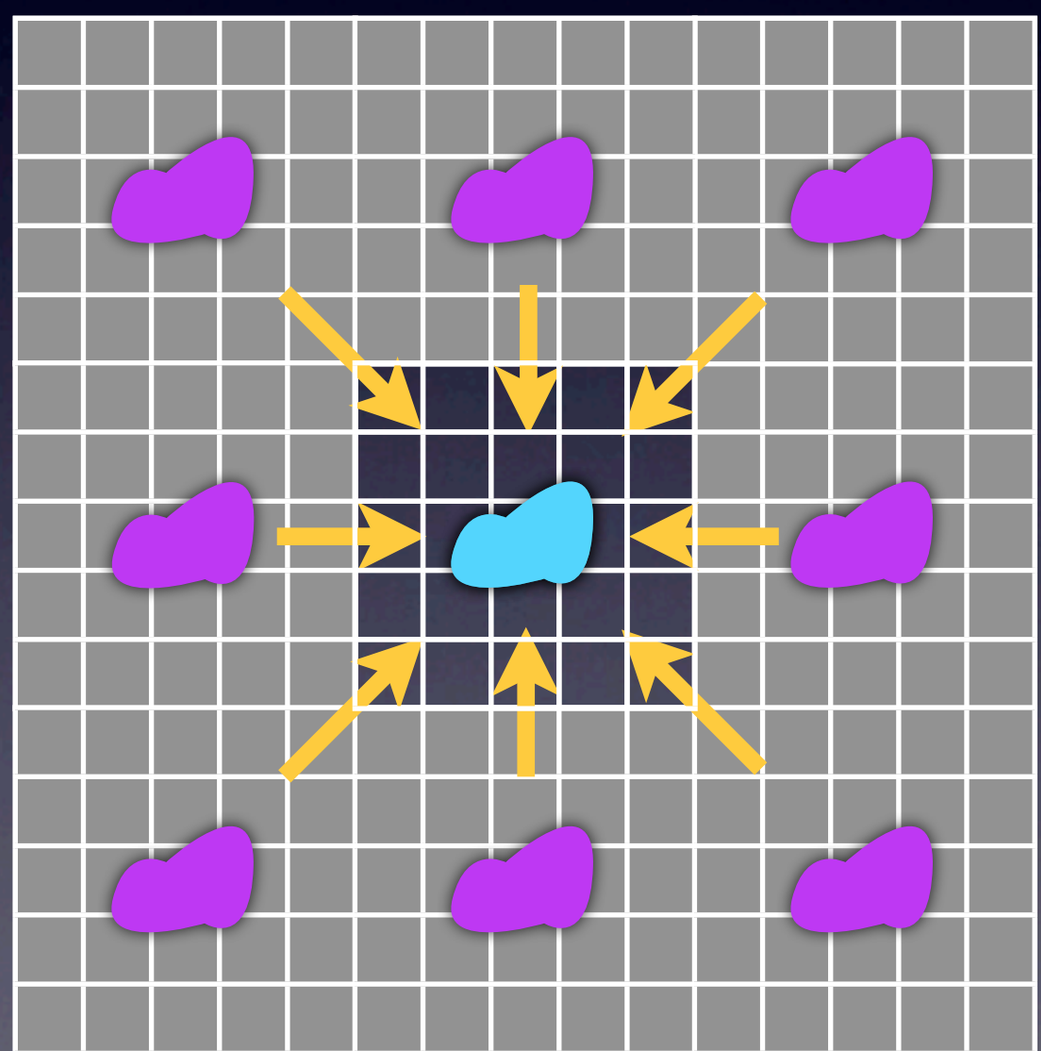


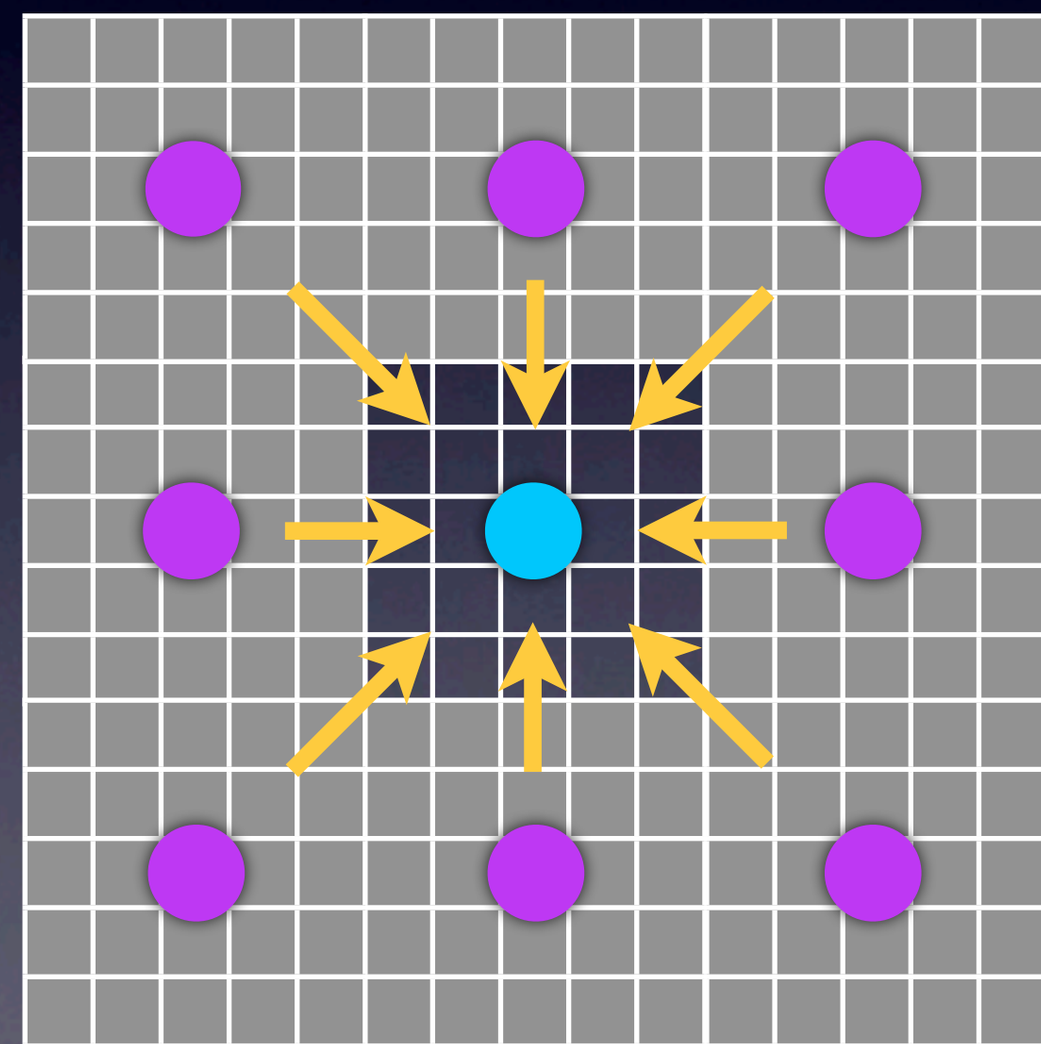
$$\phi = \phi^{\mathrm{FFT}} - \varepsilon$$



$$\phi = \phi^{\mathrm{FFT}} - \varepsilon$$

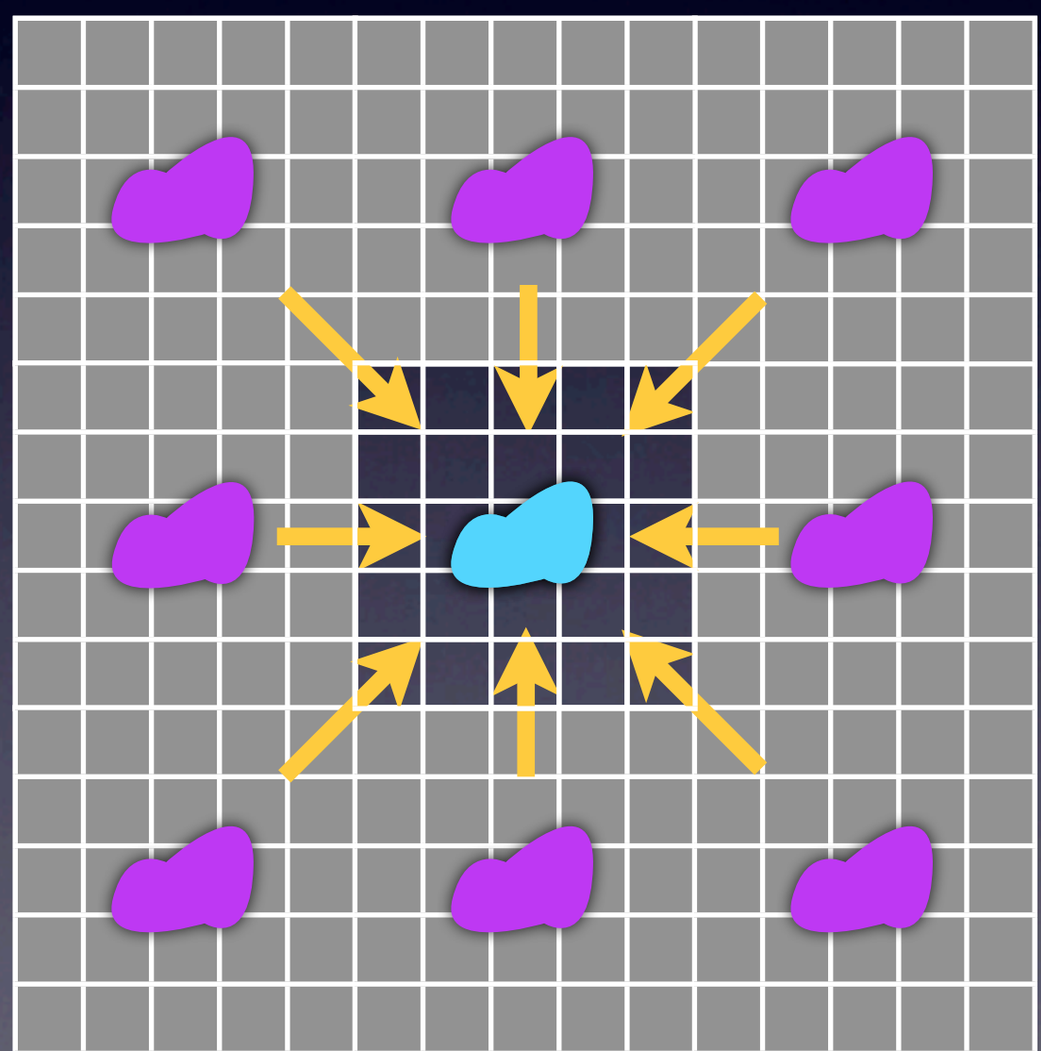
$$\varepsilon_{mono} = \phi_{mono}^{\mathrm{FFT}} - \phi_{mono}^{\mathrm{analy}}$$

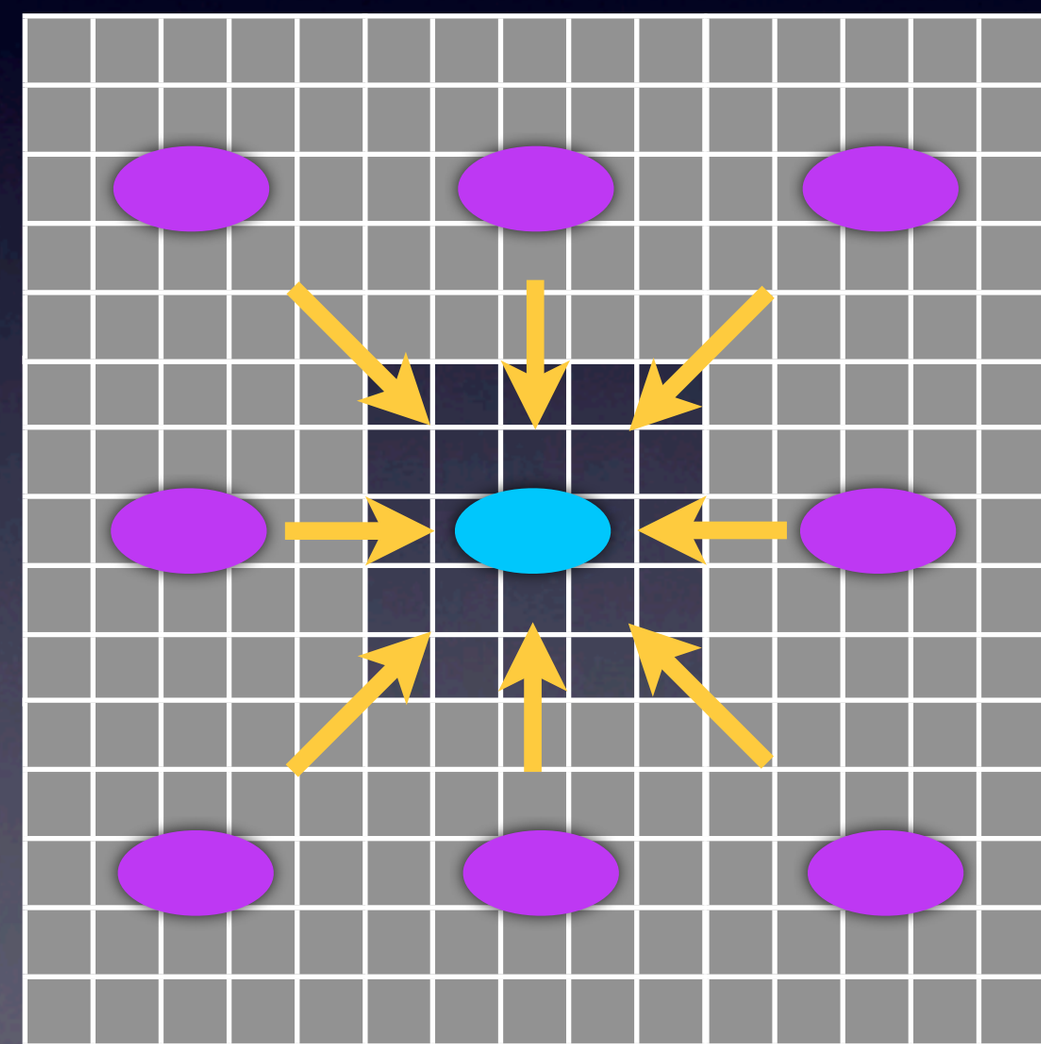




$$\phi = \phi^{\mathrm{FFT}} - \varepsilon$$

$$\varepsilon_{\mathrm{model}} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left(\phi_{lm}^{\mathrm{FFT}} - \phi_{lm}^{\mathrm{analy}} \right)$$





Error correct error

$$\phi = \phi^{\mathrm{FFT}} - \varepsilon$$

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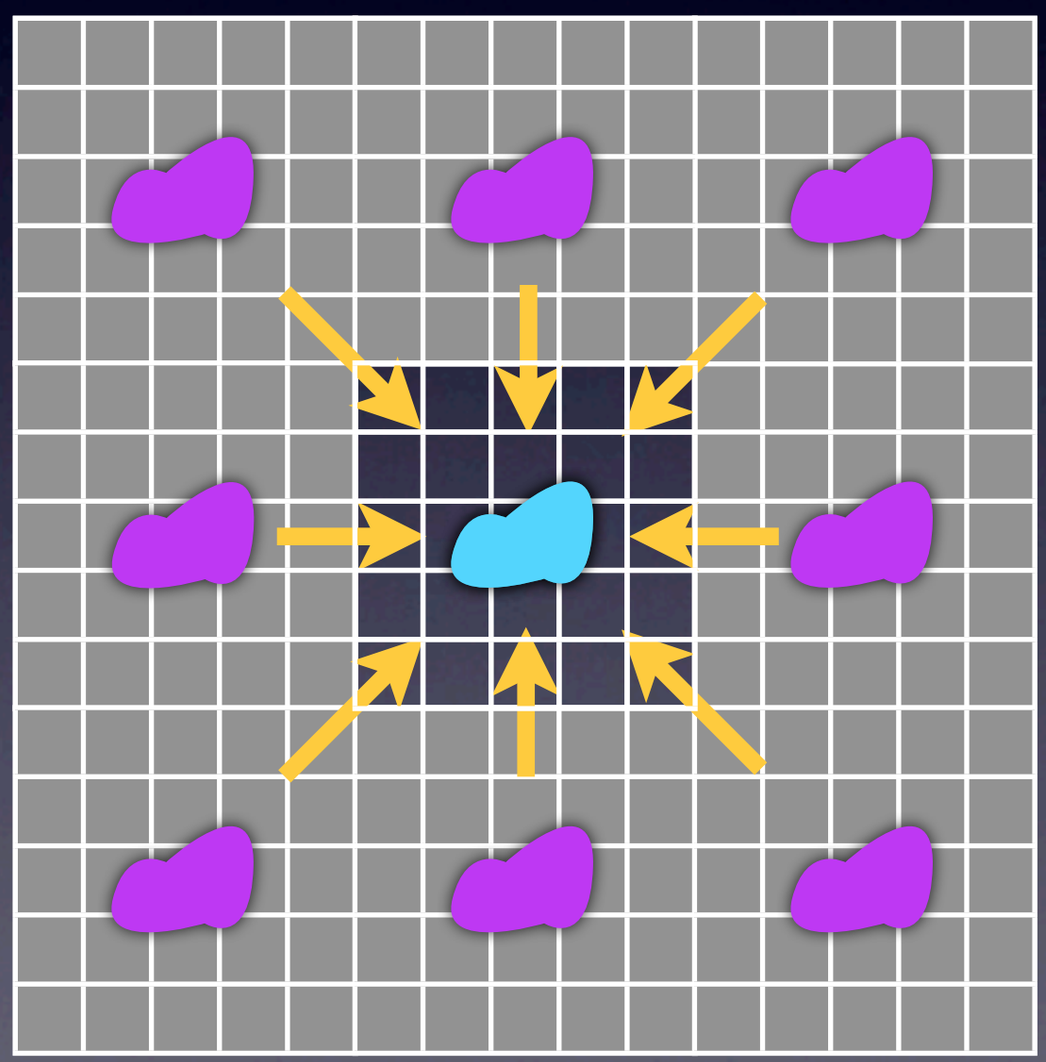
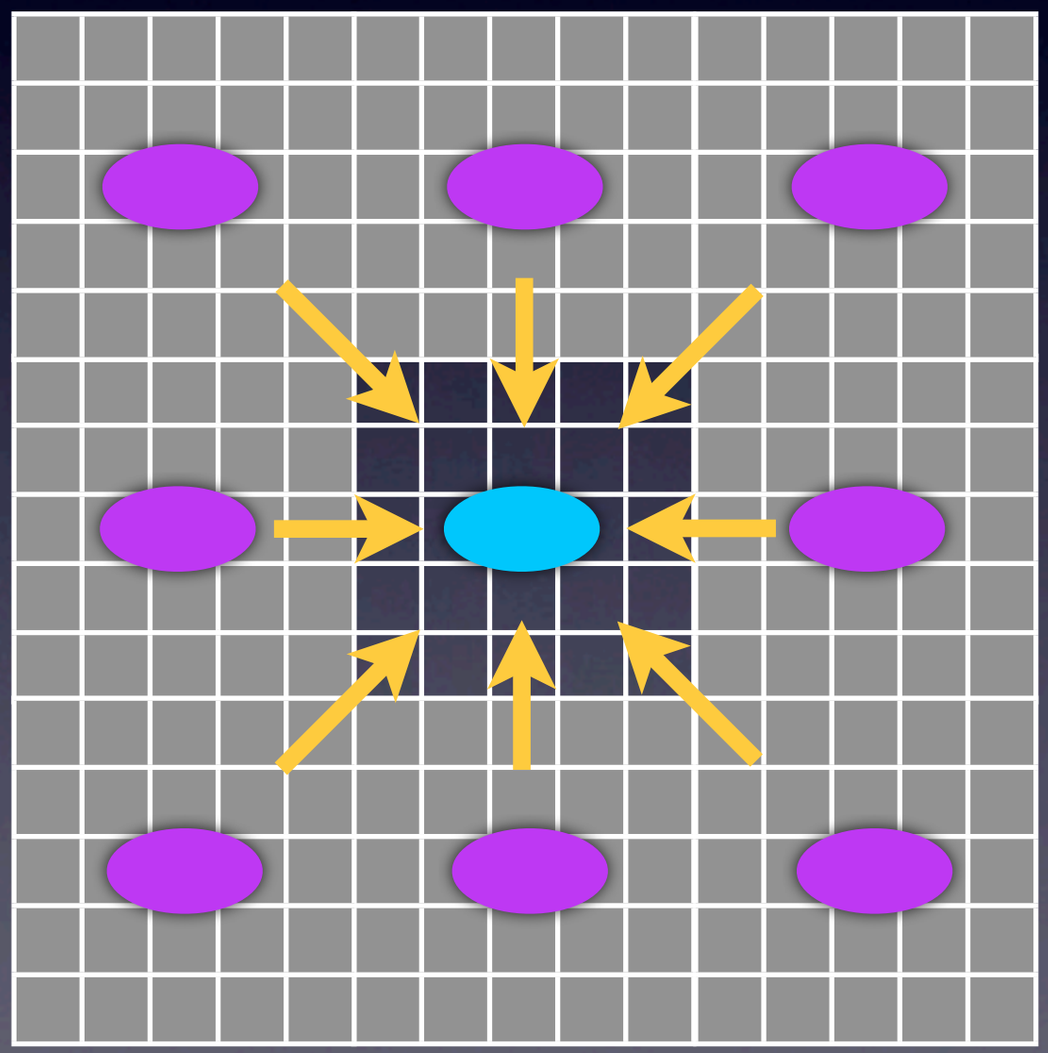
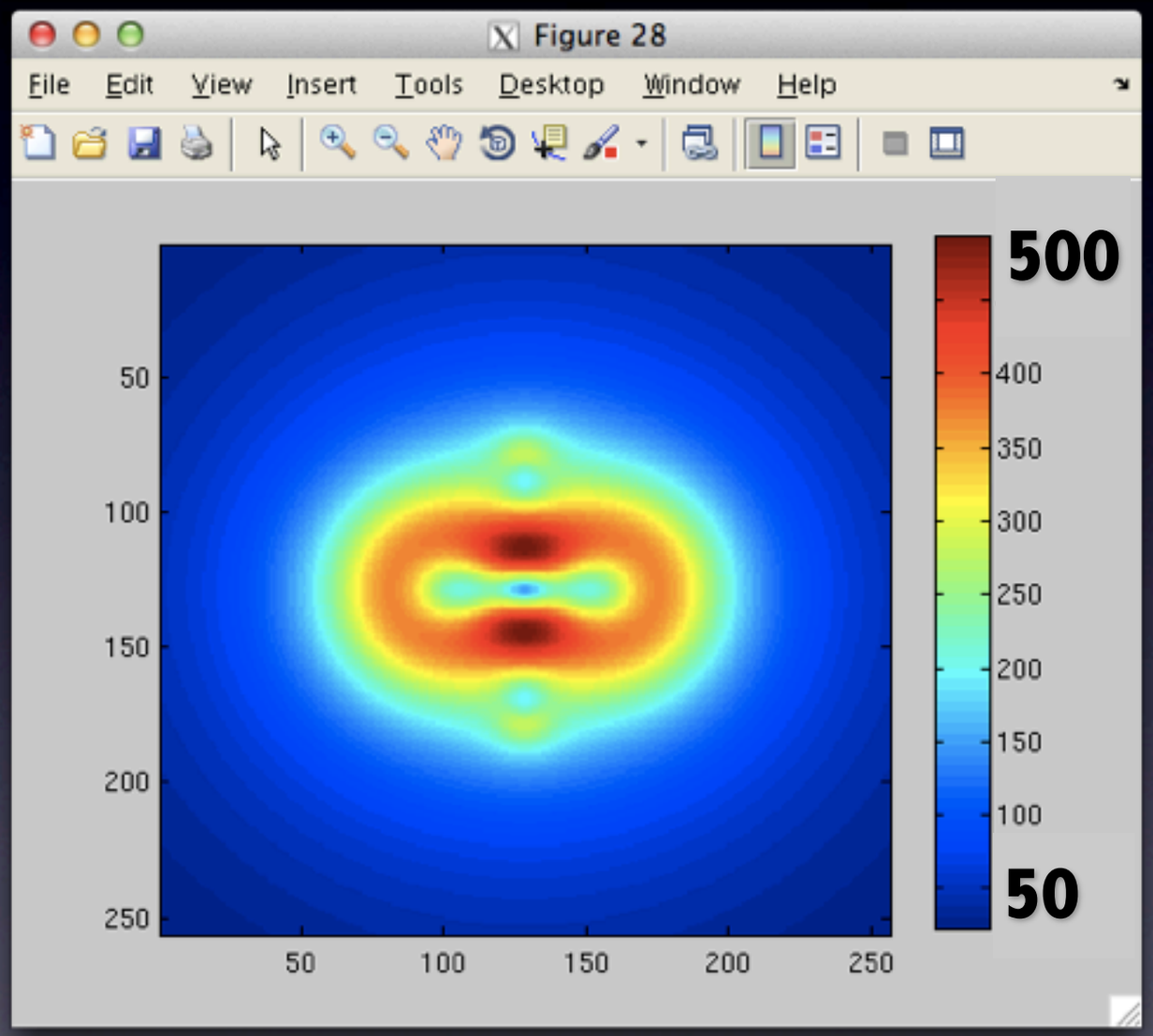




Multipole correction

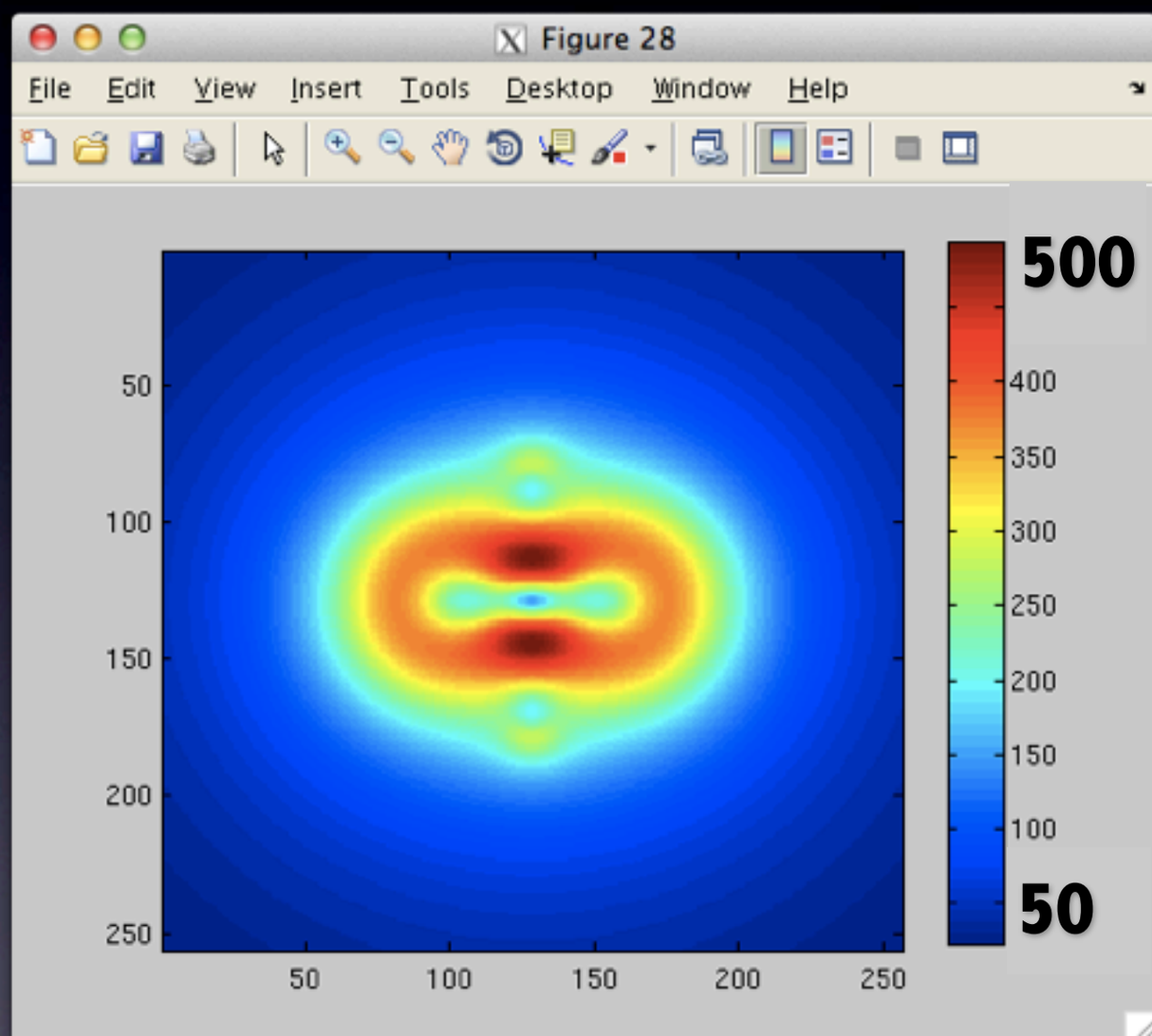
$$\left|\mathbf{F}_{\text{analy}}\right|$$

$$\varepsilon_{\text{FFT}} = \left|\mathbf{F}_{\text{FFT}}\right| - \left|\mathbf{F}_{\text{analy}}\right|$$

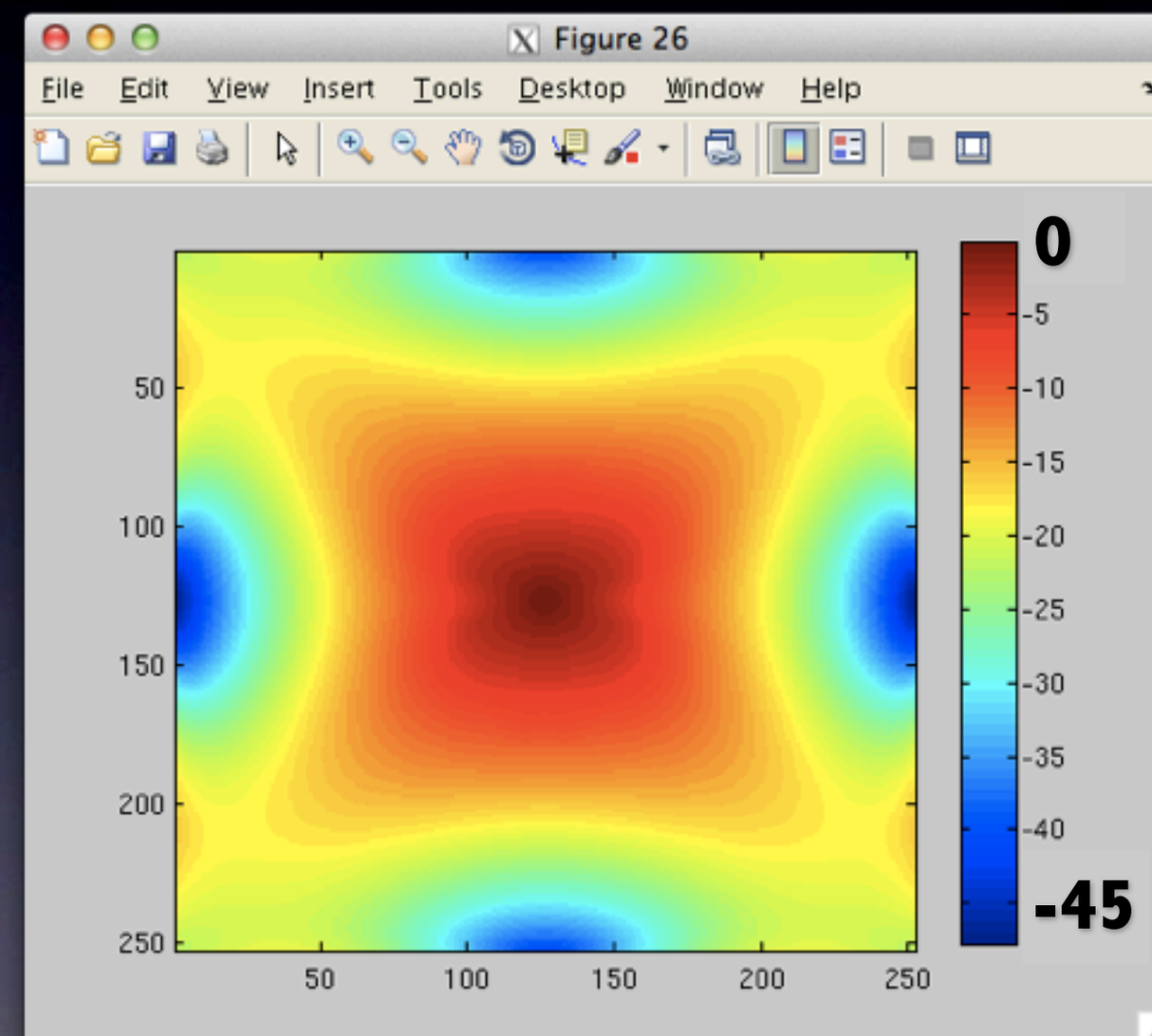


Multipole correction

$$\left|\mathbf{F}_{\text{analy}}\right|$$



$$\varepsilon_{\text{FFT}} = \left|\mathbf{F}_{\text{FFT}}\right| - \left|\mathbf{F}_{\text{analy}}\right|$$

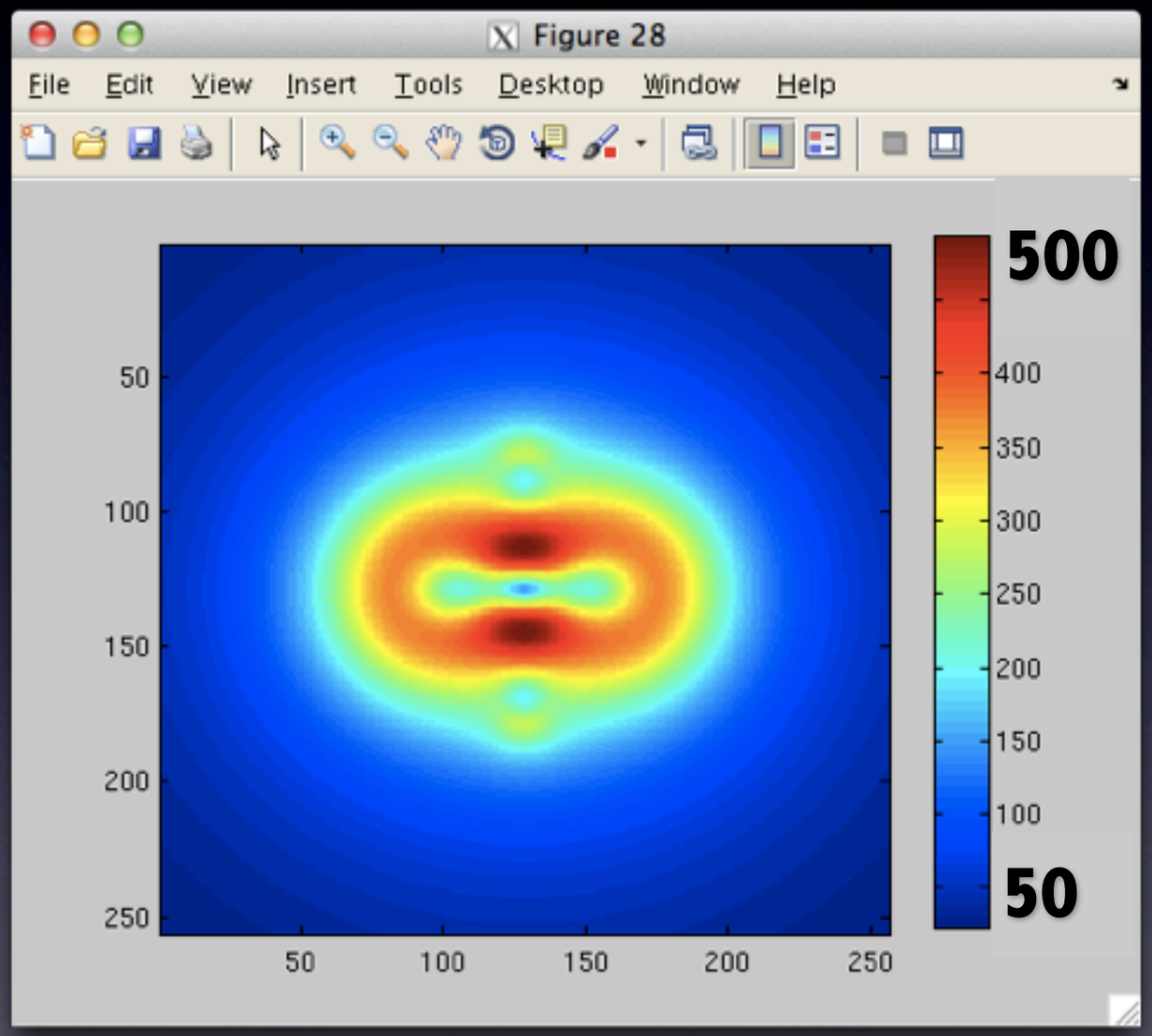


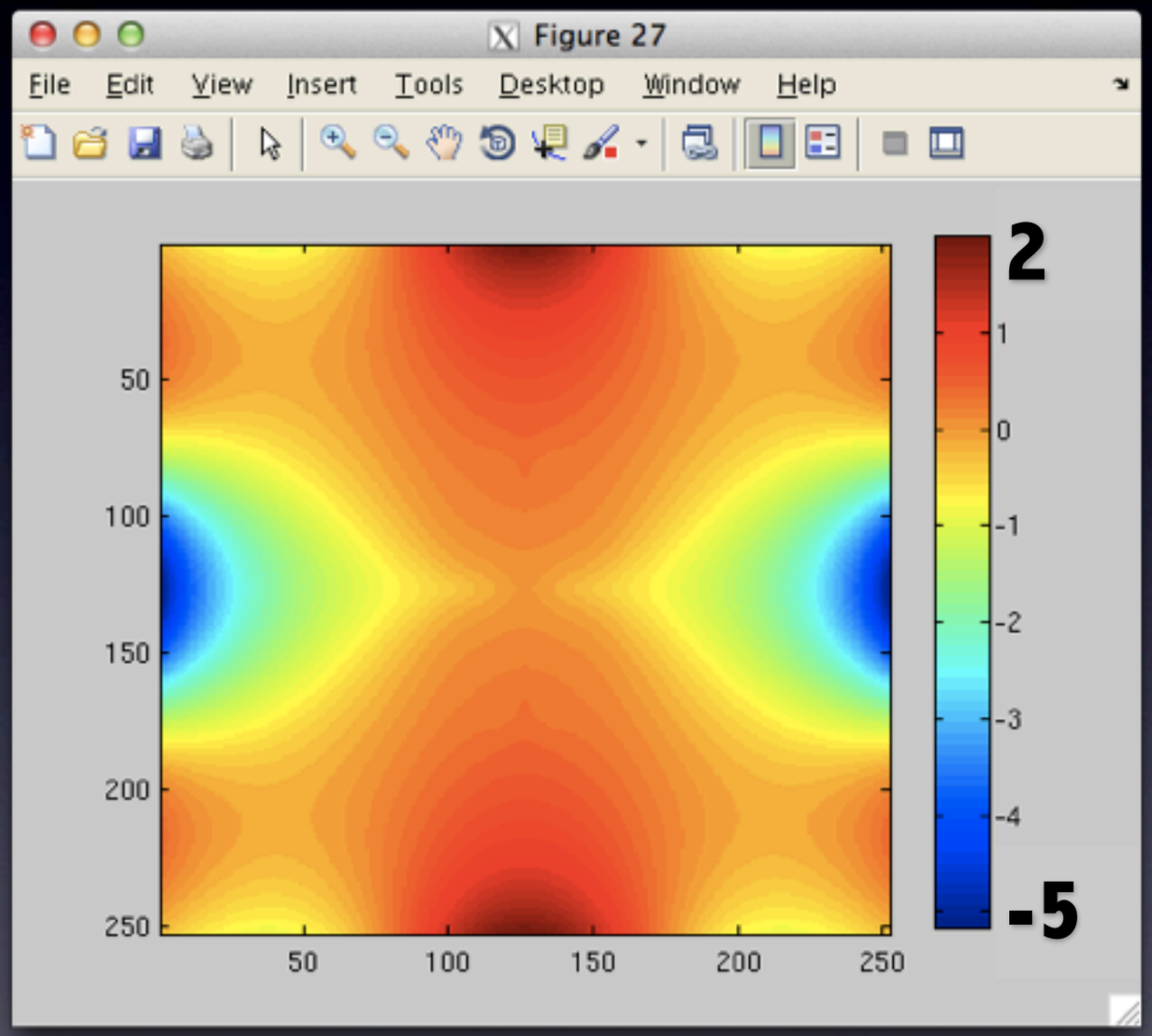
$$\frac{\max(\left|\varepsilon_{\text{FFT}}\right|)}{\max(\left|\mathbf{F}_{\text{analy}}\right|)} \sim 0.1$$

Multipole correction

$$\left|\mathbf{F}_{\text{analy}}\right|$$

$$\varepsilon_{\text{FFT}} = \left|\mathbf{F}_{\text{FFT}}\right| - \left|\mathbf{F}_{\text{analy}}\right|$$

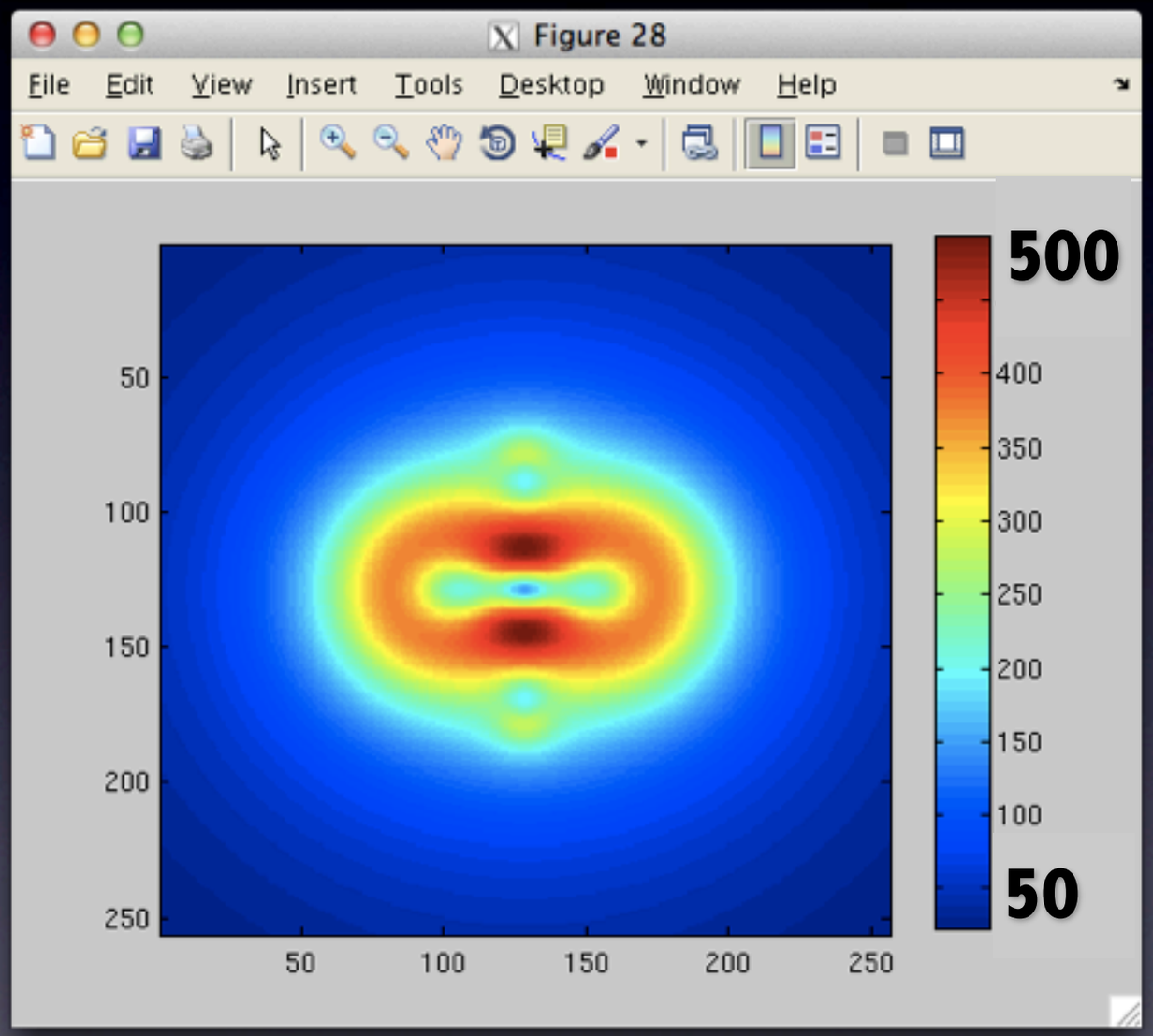




$$l = 0 \qquad \frac{\max(\left|\varepsilon_{\text{FFT}}\right|)}{\max(\left|\mathbf{F}_{\text{analy}}\right|)} \sim 10^{-2}$$

Multipole correction

$$\left|\mathbf{F}_{\text{analy}}\right|$$



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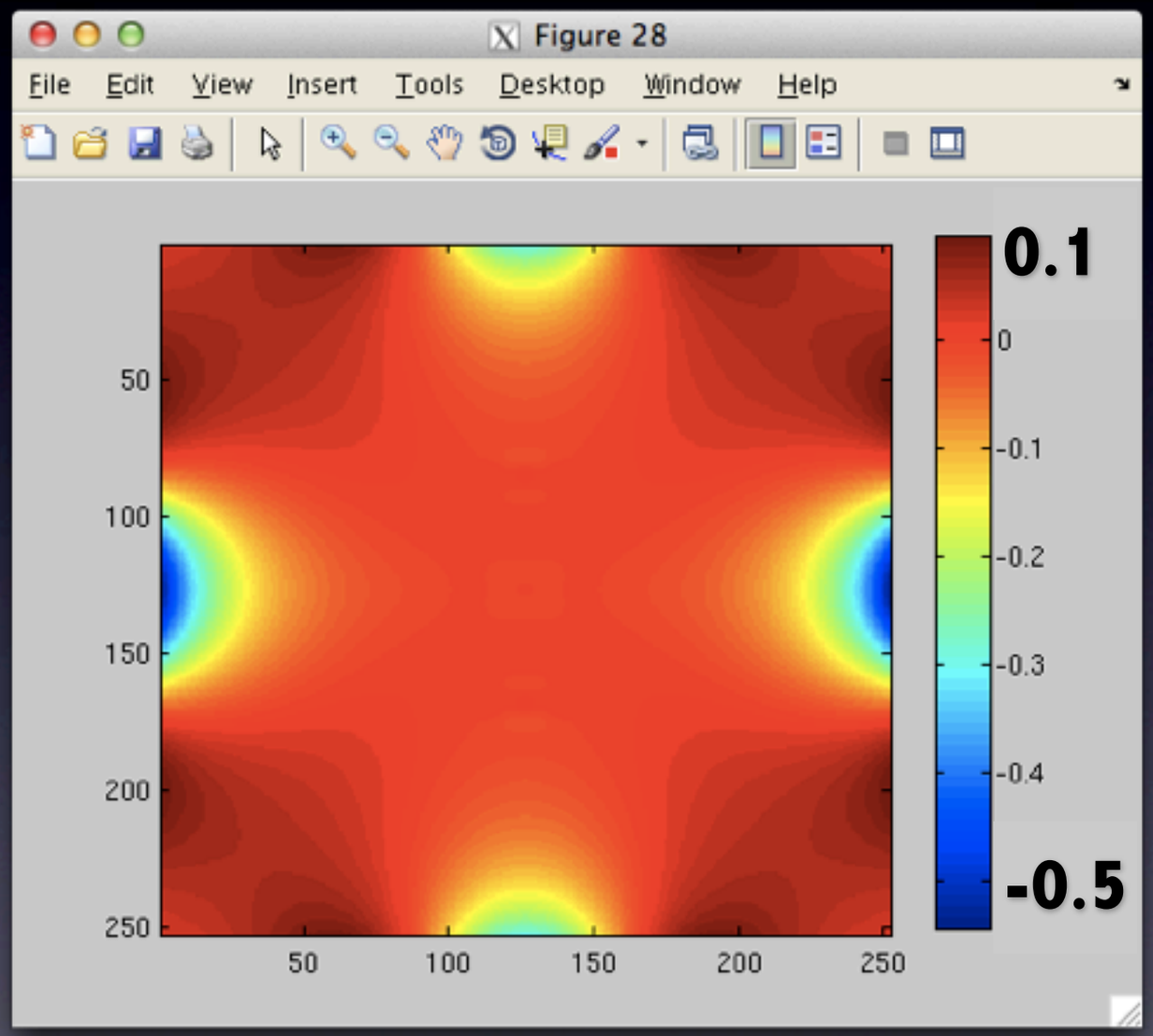
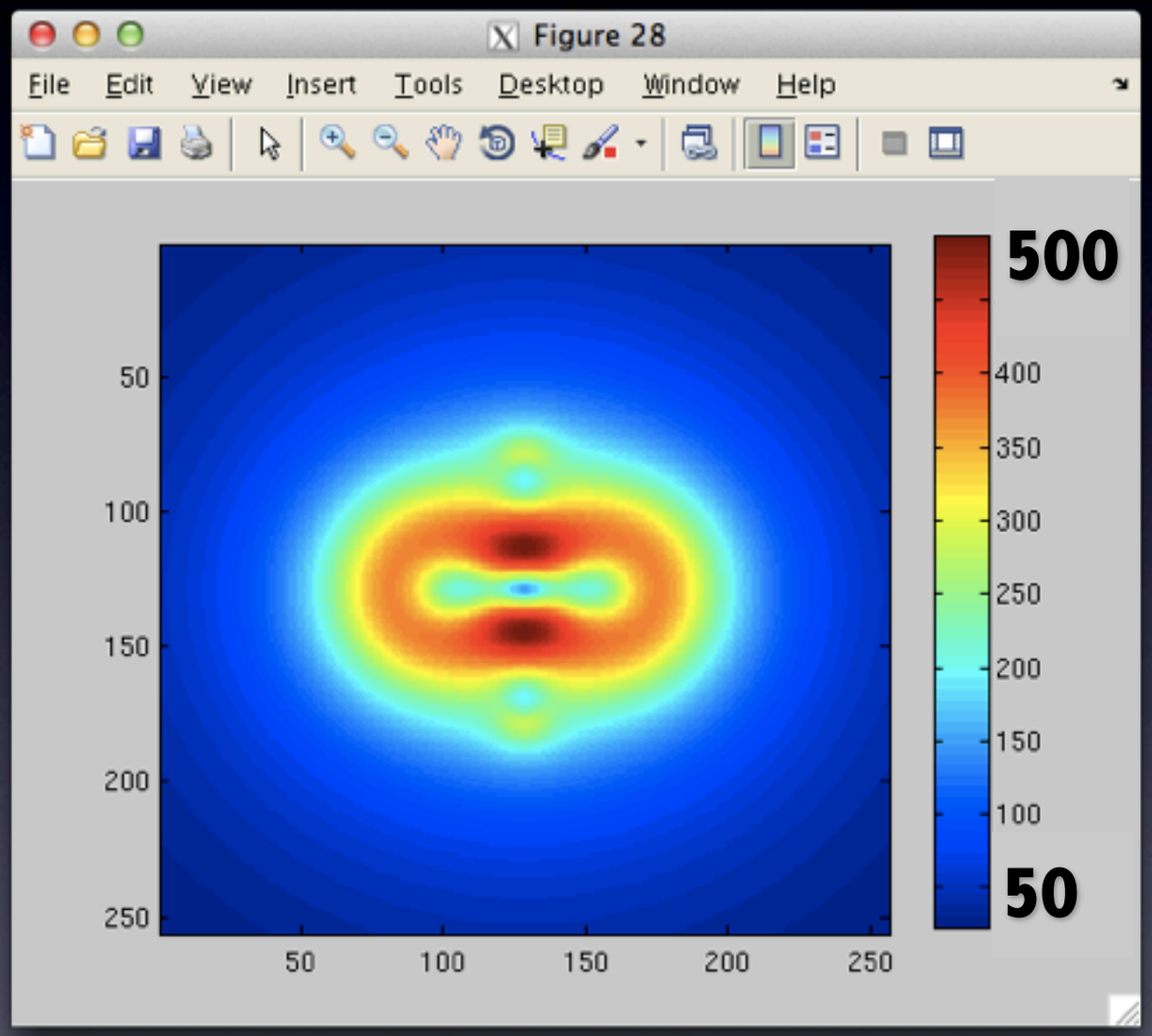


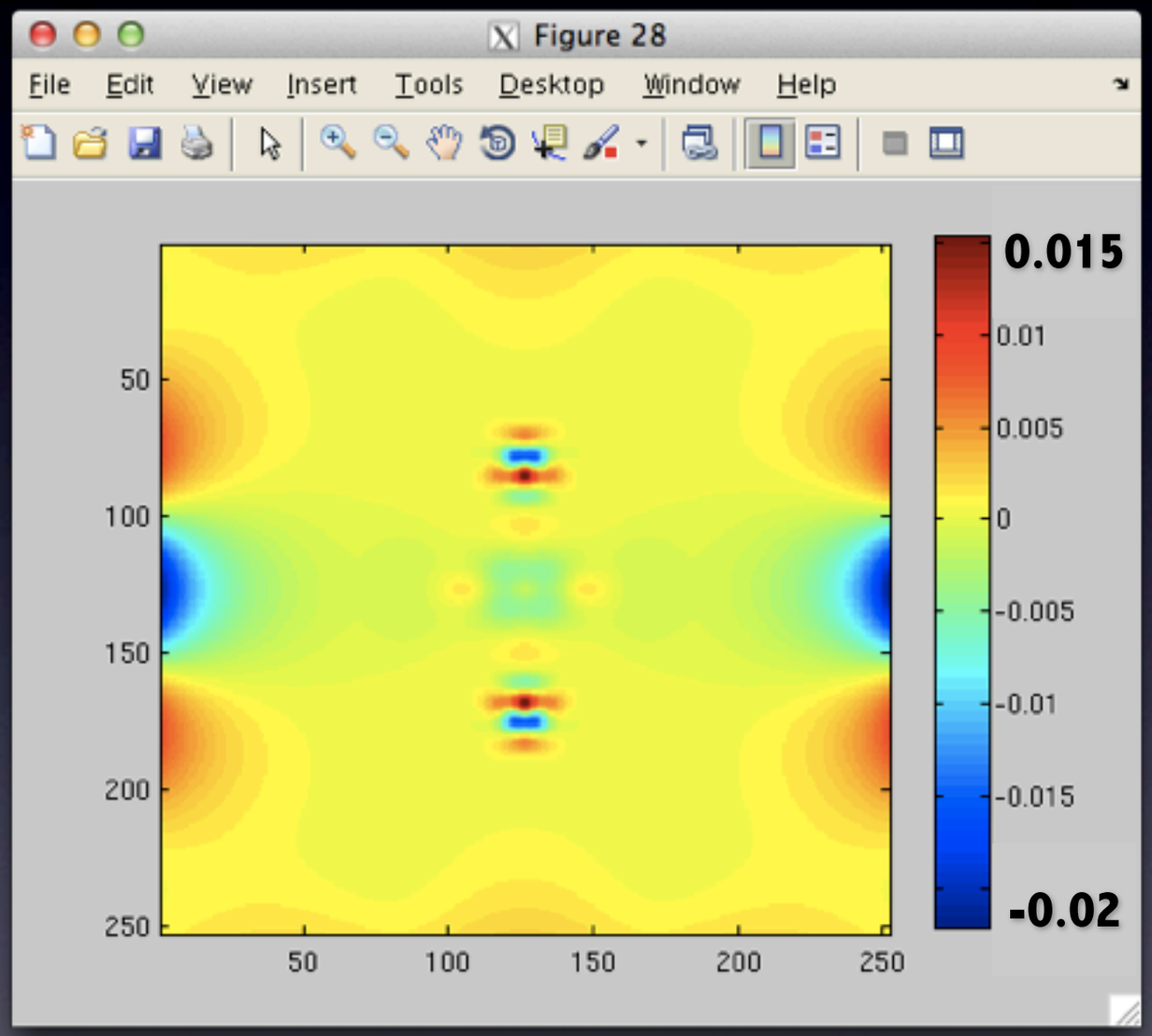
$$l = 2 \qquad \frac{\max\left(\left|\varepsilon_{\text{FFT}}\right|\right)}{\max\left(\left|\mathbf{F}_{\text{analy}}\right|\right)} \sim 10^{-3}$$

Multipole correction

$$\left|\mathbf{F}_{\text{analy}}\right|$$

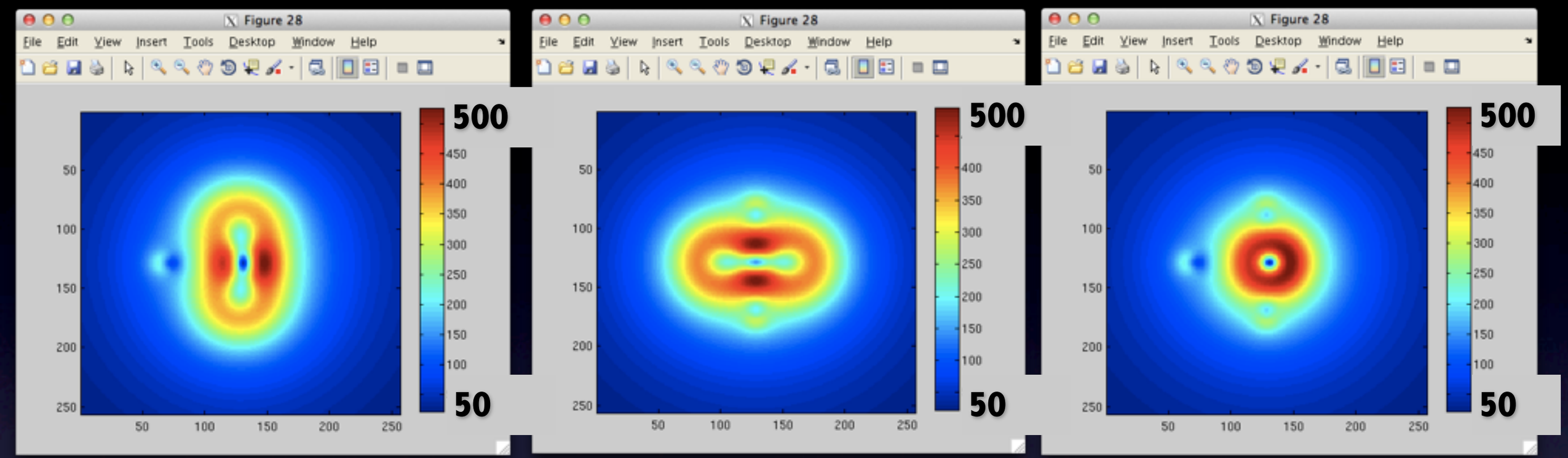
$$\varepsilon_{\text{FFT}} = \left|\mathbf{F}_{\text{FFT}}\right| - \left|\mathbf{F}_{\text{analy}}\right|$$



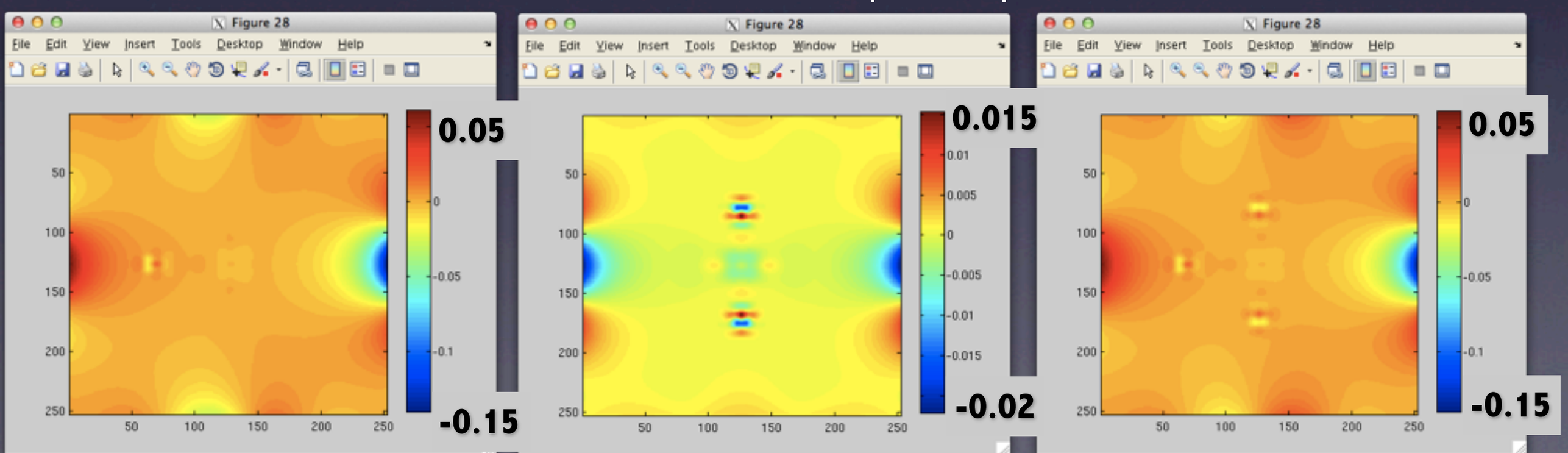


$$l = 4 \qquad \frac{\max(\left|\varepsilon_{\text{FFT}}\right|)}{\max(\left|\mathbf{F}_{\text{analy}}\right|)} \sim 4 \cdot 10^{-5}$$

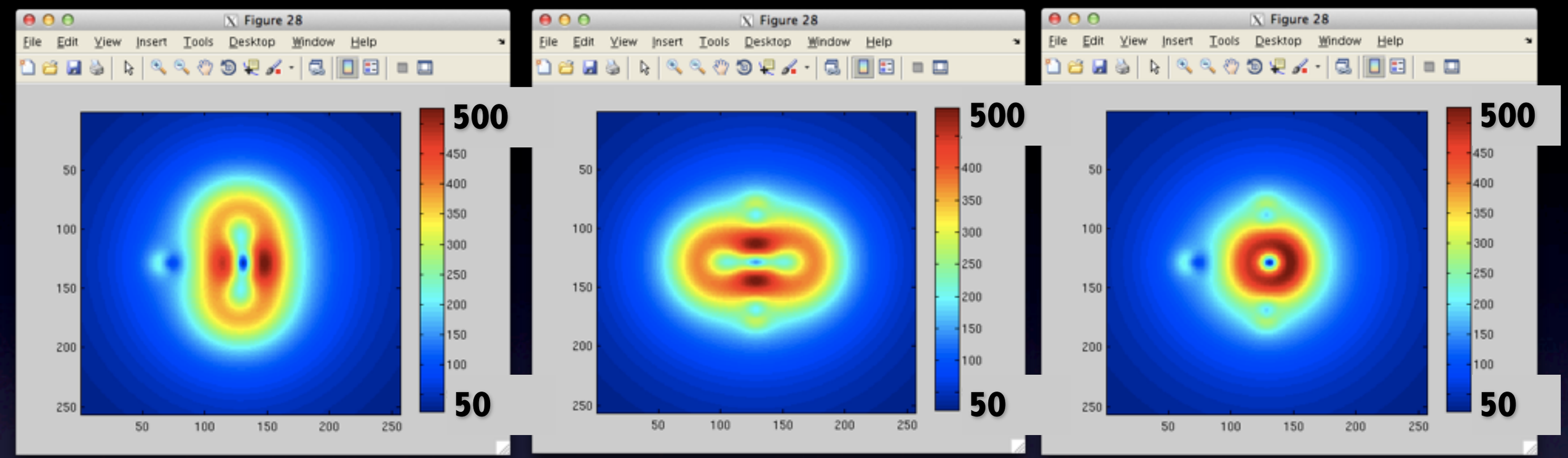
$$\left|\mathbf{F}_{\text{analy}}\right|$$



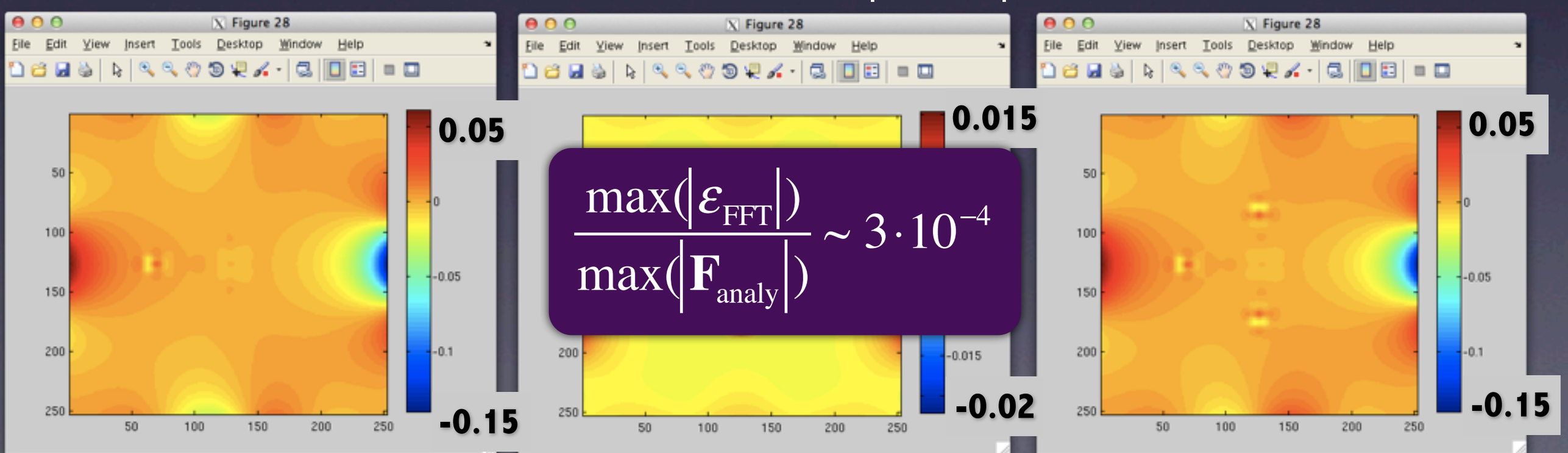
$$\varepsilon_{\text{FFT}} = \left|\mathbf{F}_{\text{FFT}}\right| - \left|\mathbf{F}_{\text{analy}}\right|$$



$$\left|\mathbf{F}_{\text{analy}}\right|$$



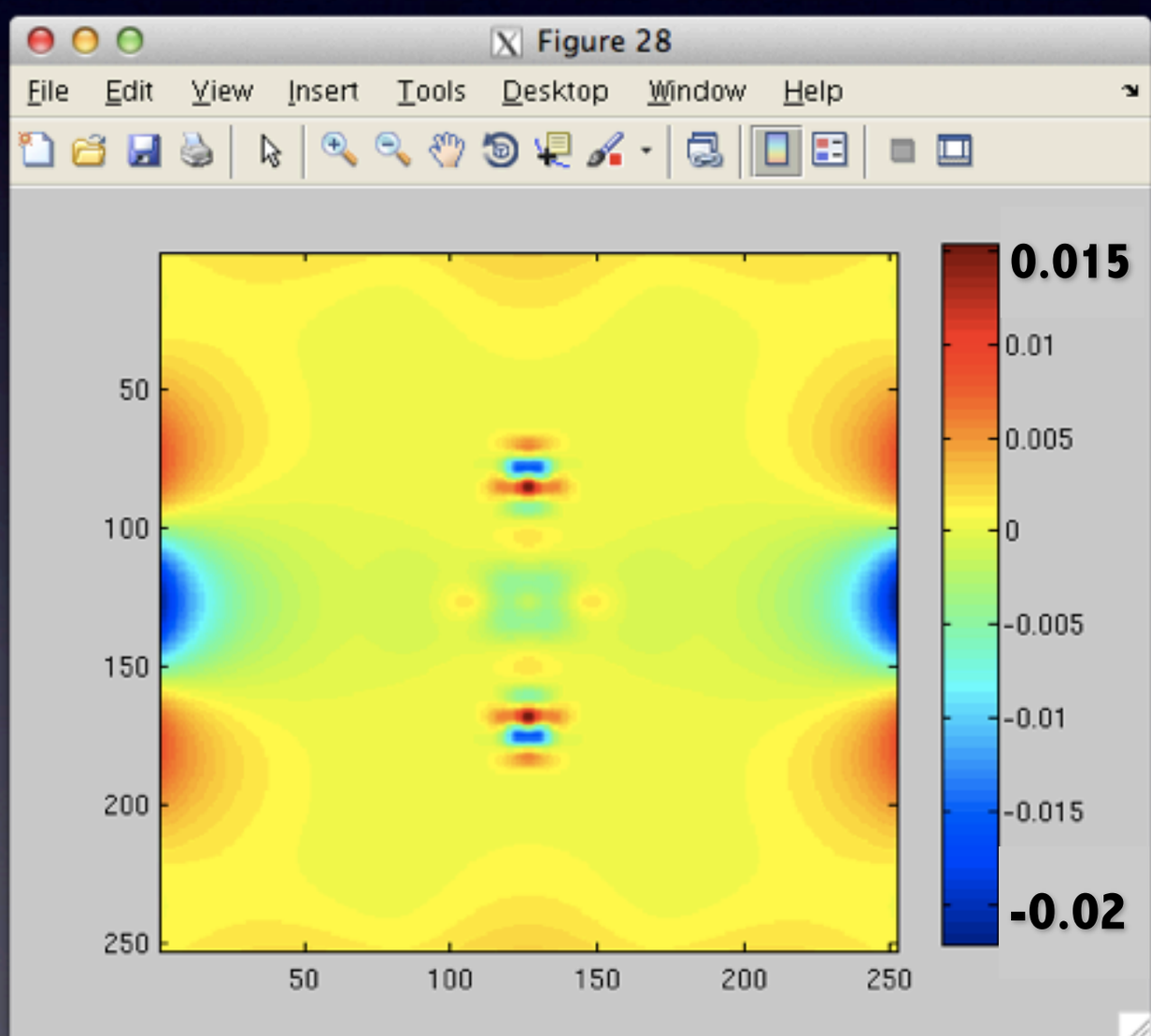
$$\varepsilon_{\text{FFT}} = \left|\mathbf{F}_{\text{FFT}}\right| - \left|\mathbf{F}_{\text{analy}}\right|$$

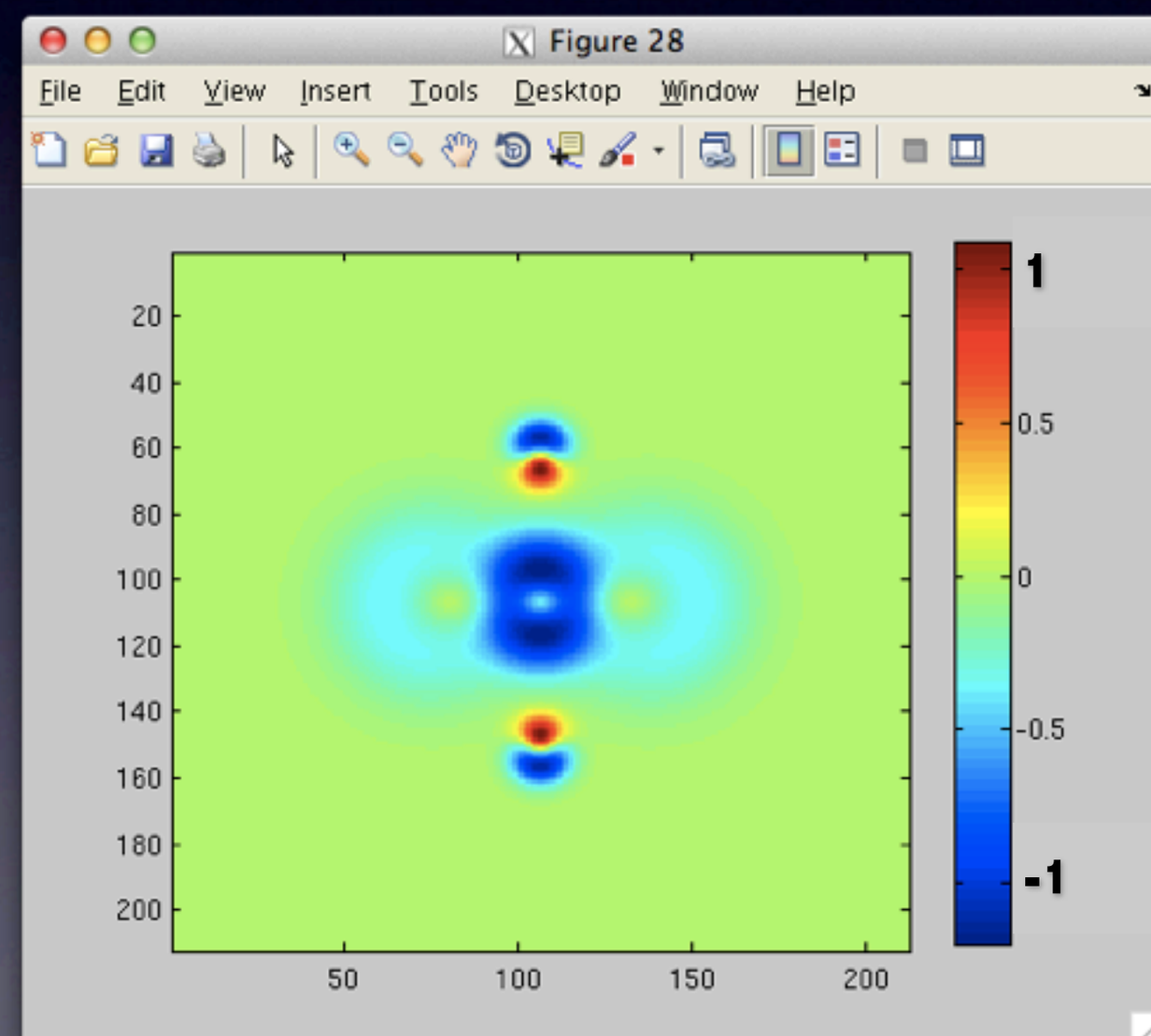


$$\frac{\max(\left|\varepsilon_{\text{FFT}}\right|)}{\max(\left|\mathbf{F}_{\text{analy}}\right|)} \sim 3 \cdot 10^{-4}$$

Multipole Correction v.s. Green's Function

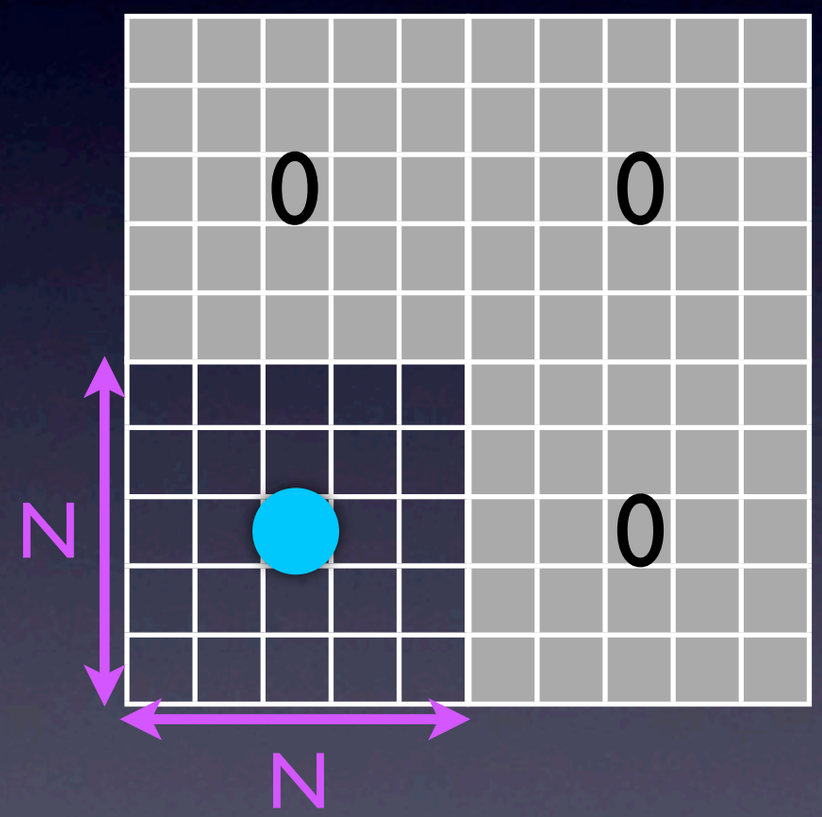
$$\varepsilon_{\mathrm{FFT}} = \left|\mathbf{F}_{\mathrm{FFT}}\right| - \left|\mathbf{F}_{\mathrm{analy}}\right|$$

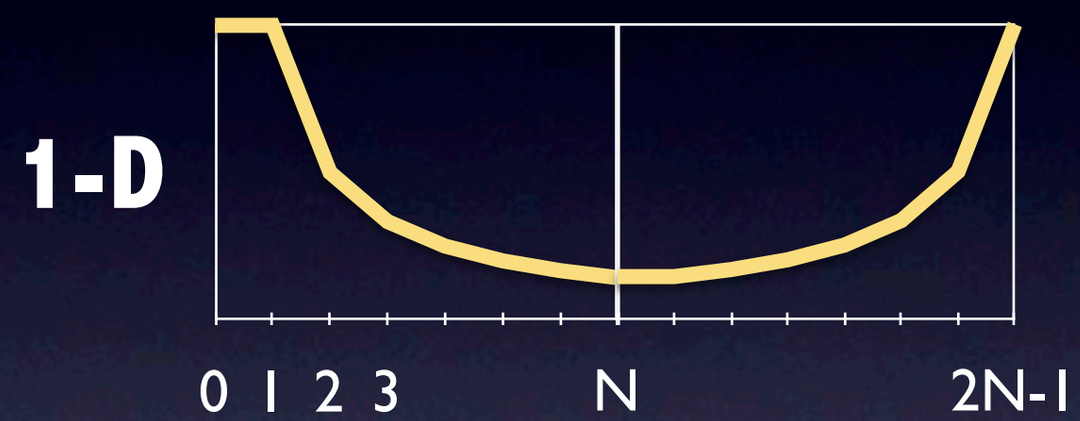




Why?

Green's Function

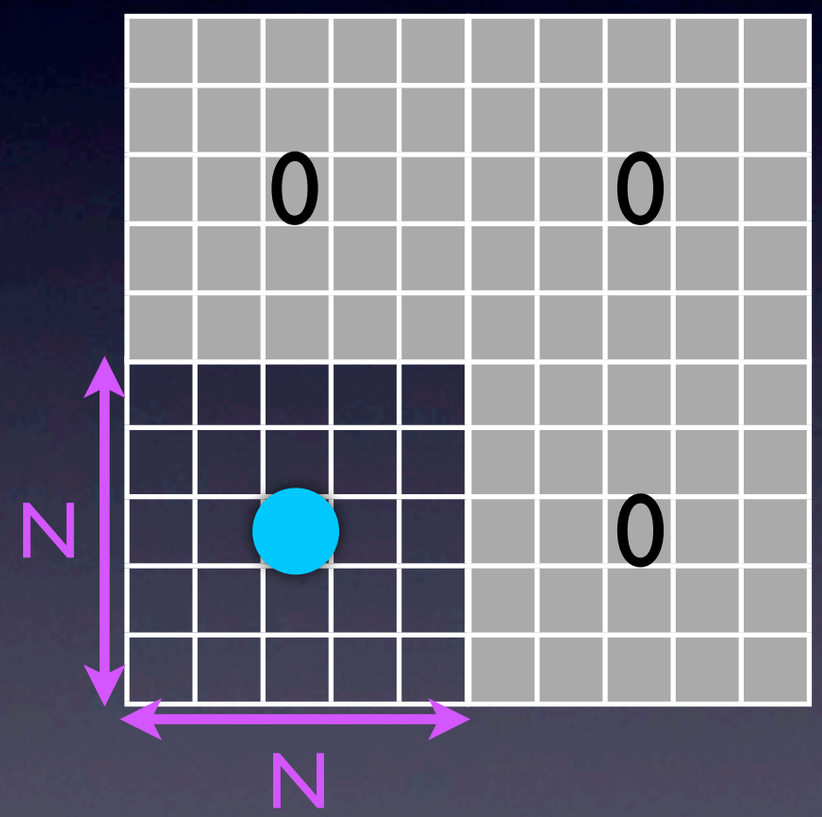


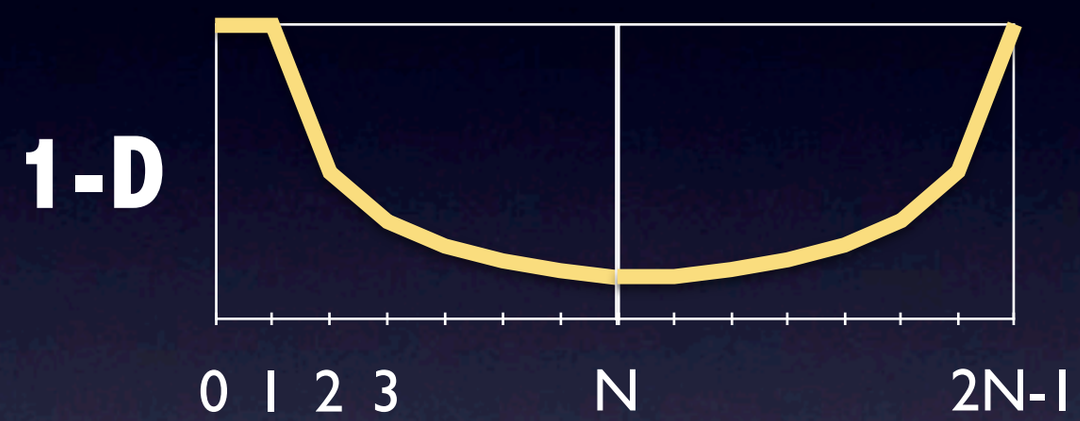


$$G_i = -\frac{1}{4\pi\sqrt{i}} = G_{2N-i} \qquad 1 \le i \le N$$

$$G_0 = -\frac{1}{4\pi}$$

Green's Function

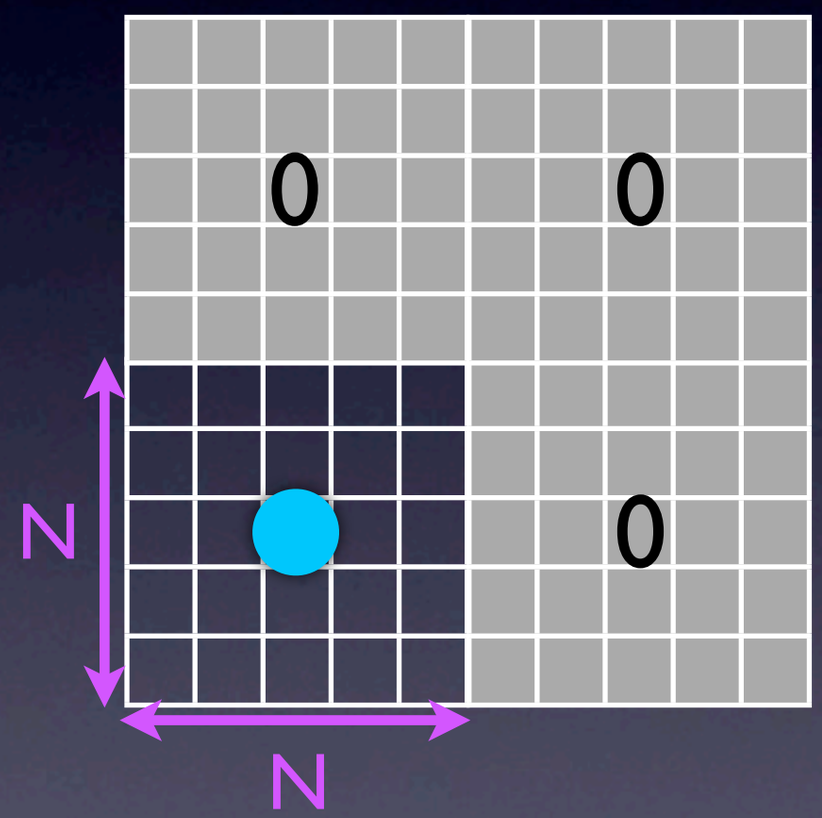


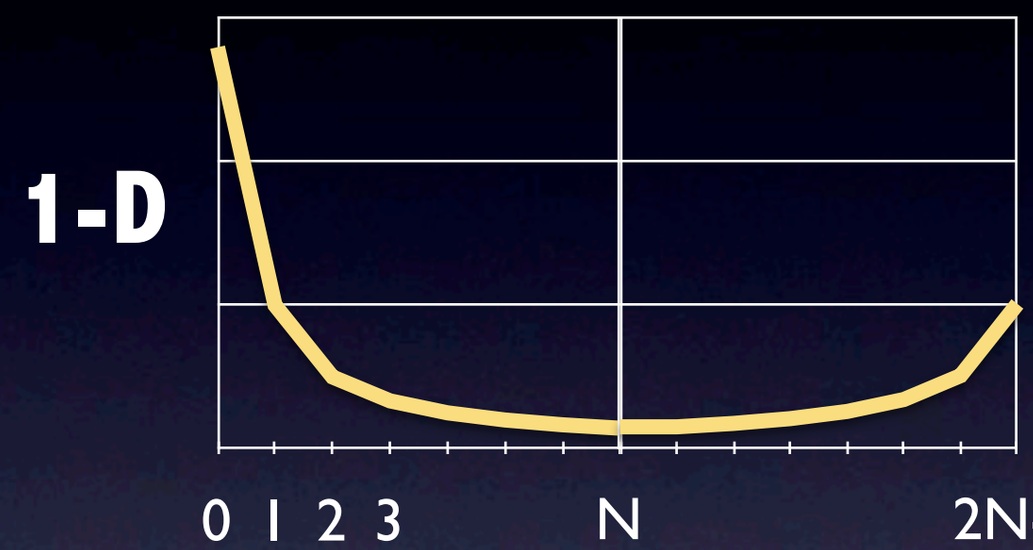


$$G_i = -\frac{1}{4\pi\sqrt{i}} = G_{2N-i} \qquad 1 \le i \le N$$

$$G_0 = -\frac{1}{4\pi}$$

Green's Function

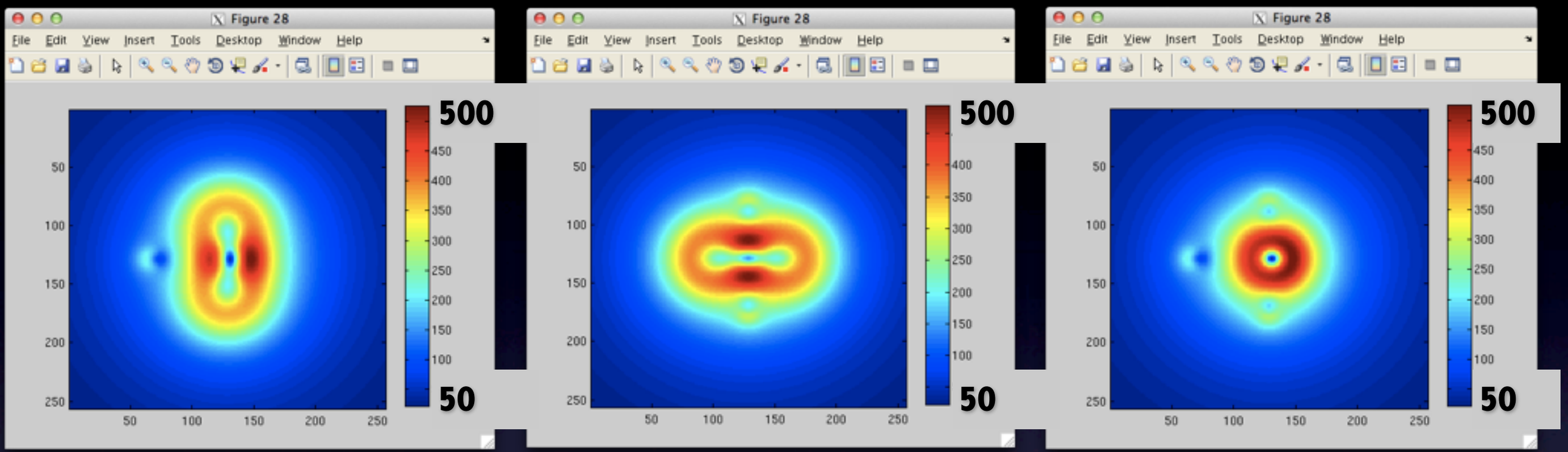




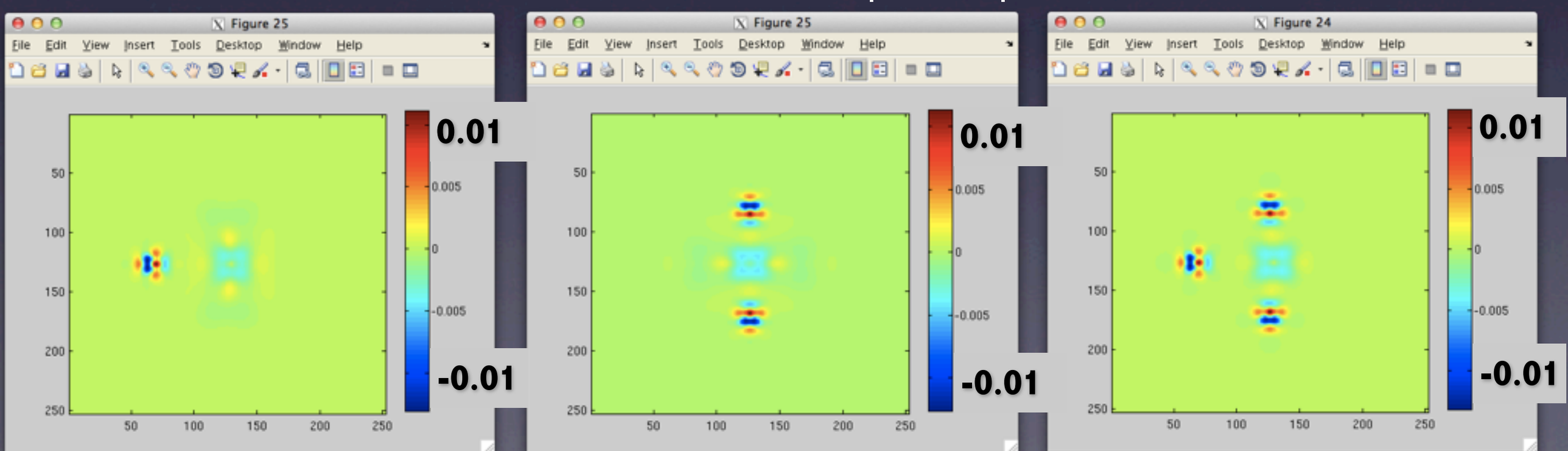
$$G_i = -\frac{1}{4\pi\sqrt{i}} = G_{2N-i} \qquad 1 \le i \le N$$

$$G_0 = -\frac{2.8362}{4\pi}$$

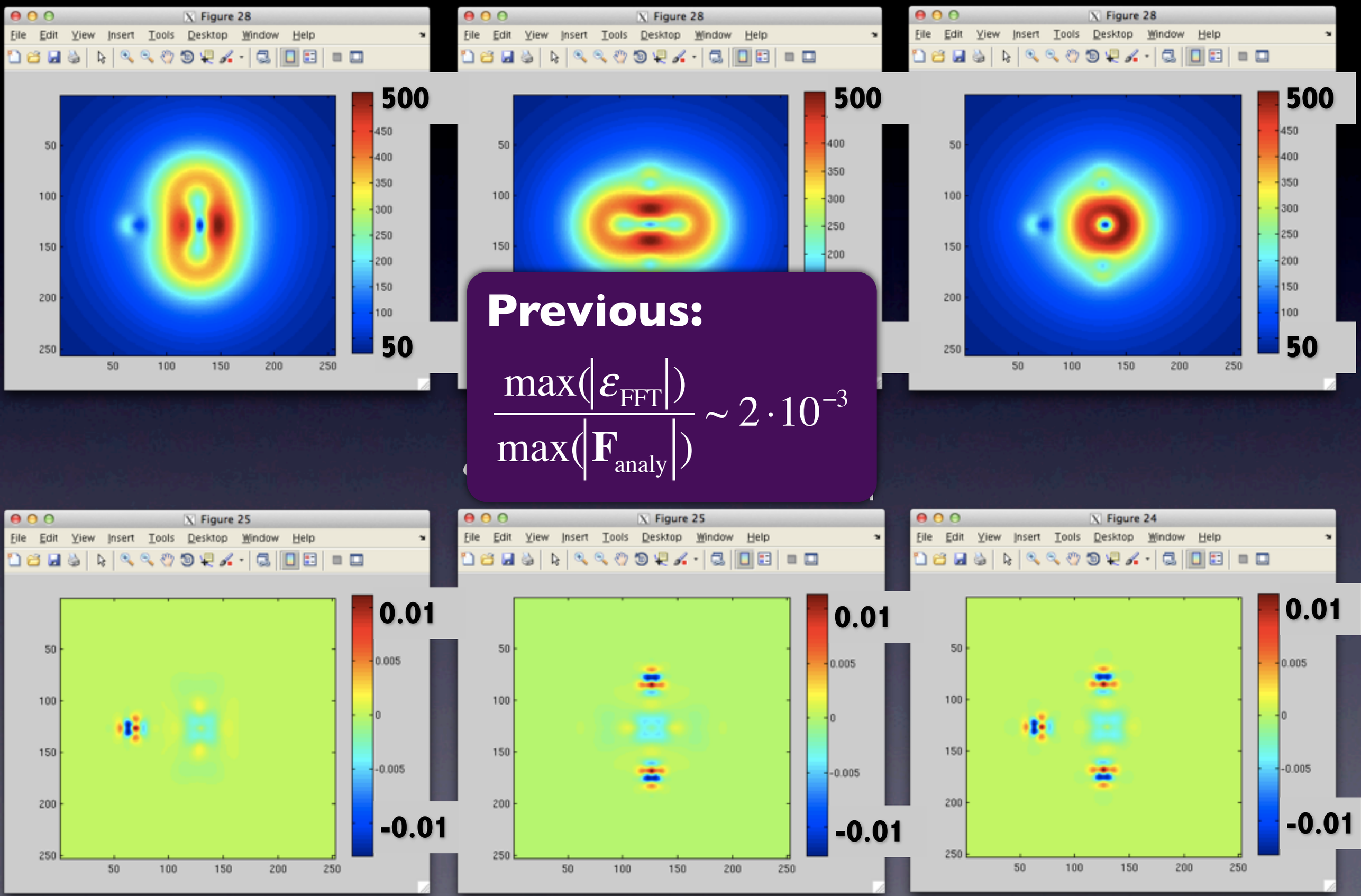
$$\left|\mathbf{F}_{\text{analy}}\right|$$



$$\varepsilon_{\text{FFT}} = \left|\mathbf{F}_{\text{FFT}}\right| - \left|\mathbf{F}_{\text{analy}}\right|$$



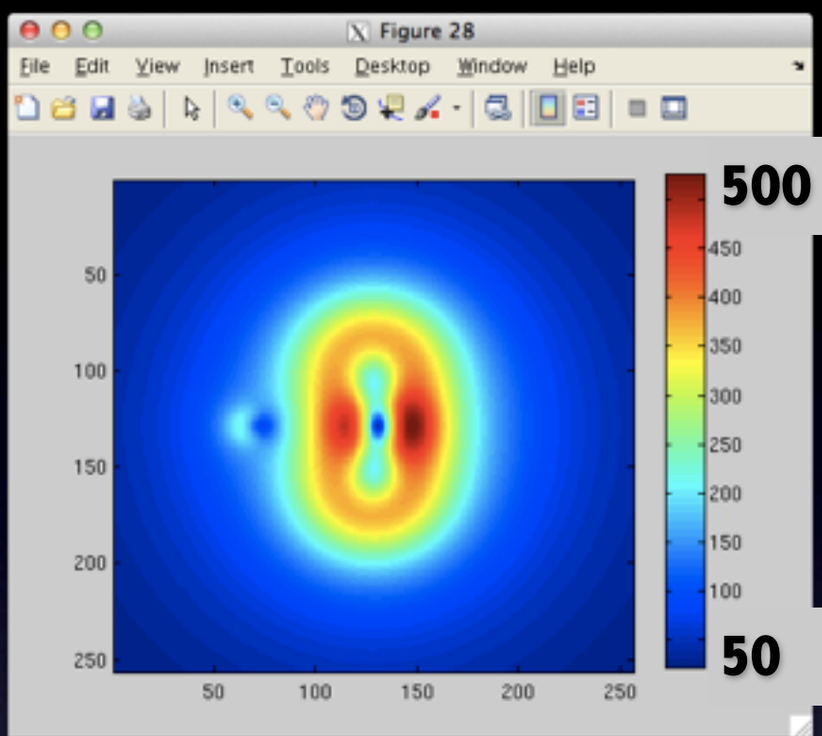
$$\left|\mathbf{F}_{\text{analy}}\right|$$

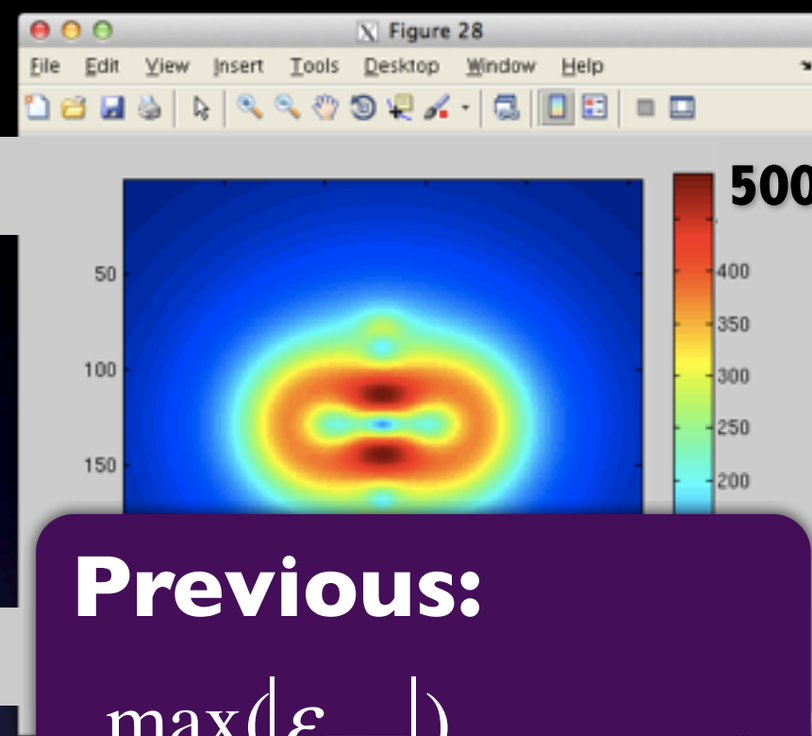


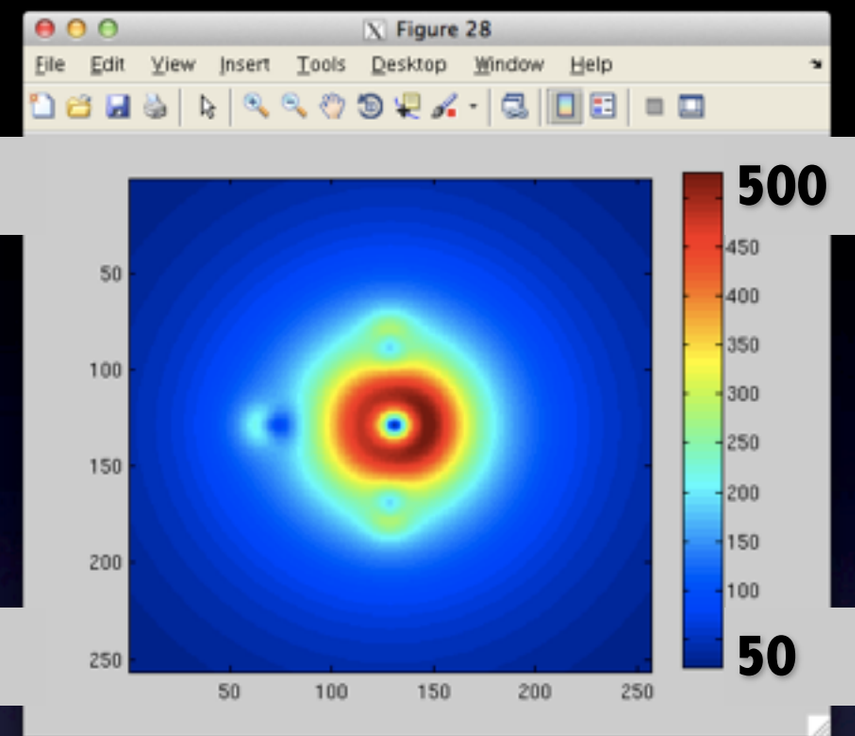
Previous:

$$\frac{\max(|\varepsilon_{\text{FFT}}|)}{\max(|\mathbf{F}_{\text{analy}}|)} \sim 2 \cdot 10^{-3}$$

$$\left|\mathbf{F}_{\text{analy}}\right|$$

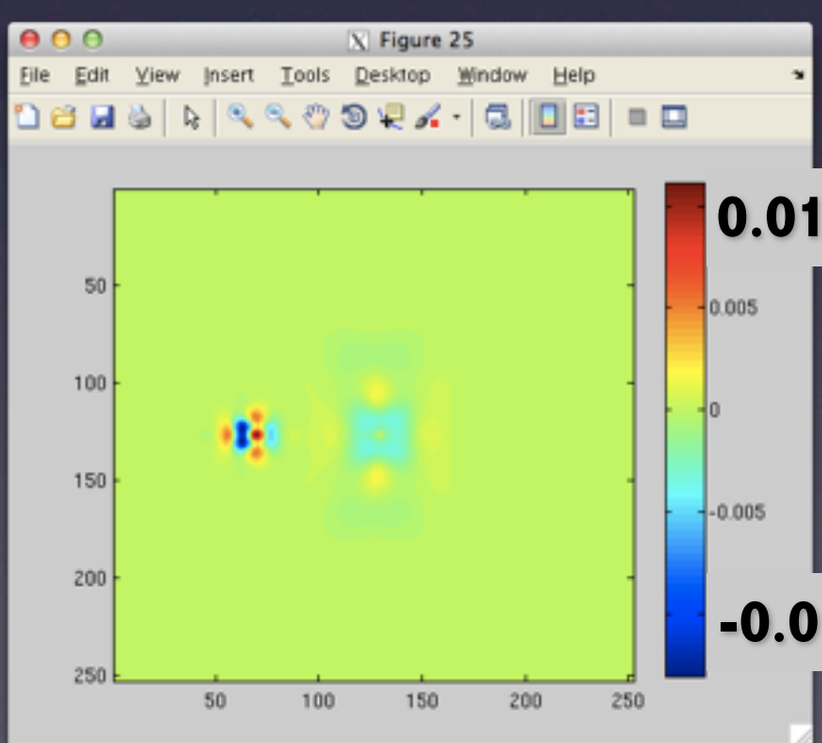


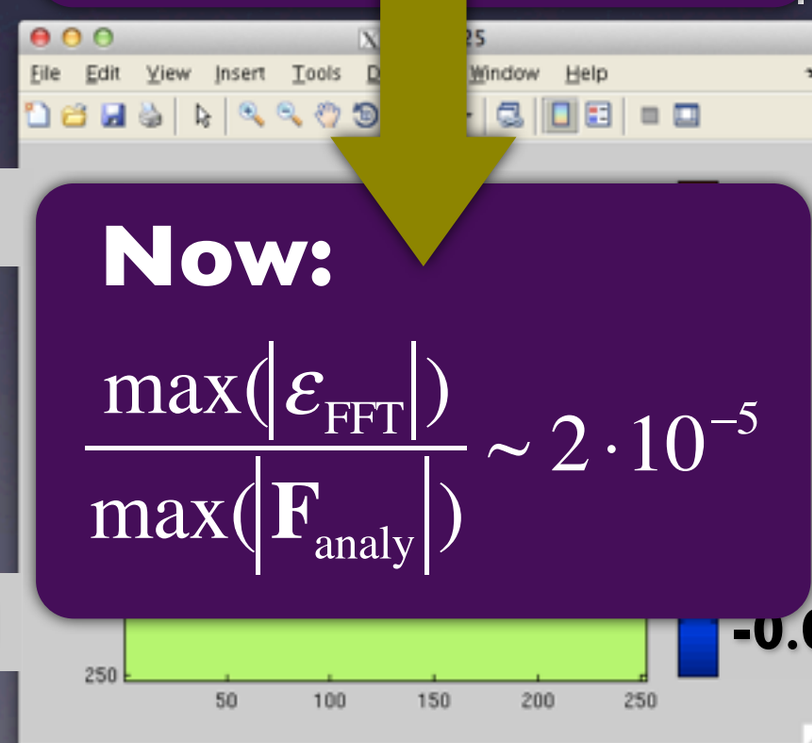


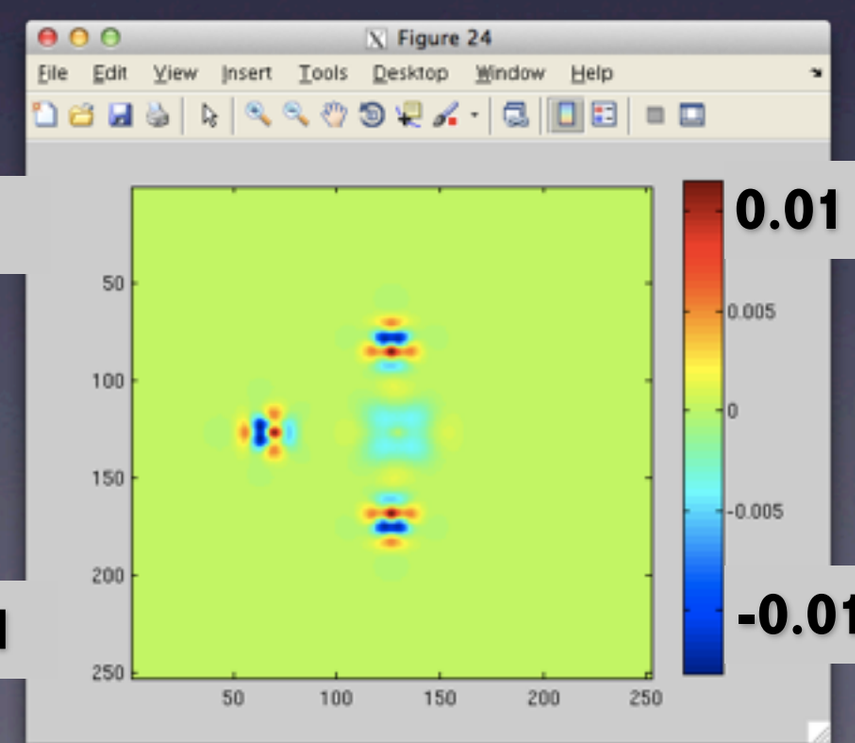


Previous:

$$\frac{\max(|\varepsilon_{\text{FFT}}|)}{\max(|\mathbf{F}_{\text{analy}}|)} \sim 2\cdot 10^{-3}$$





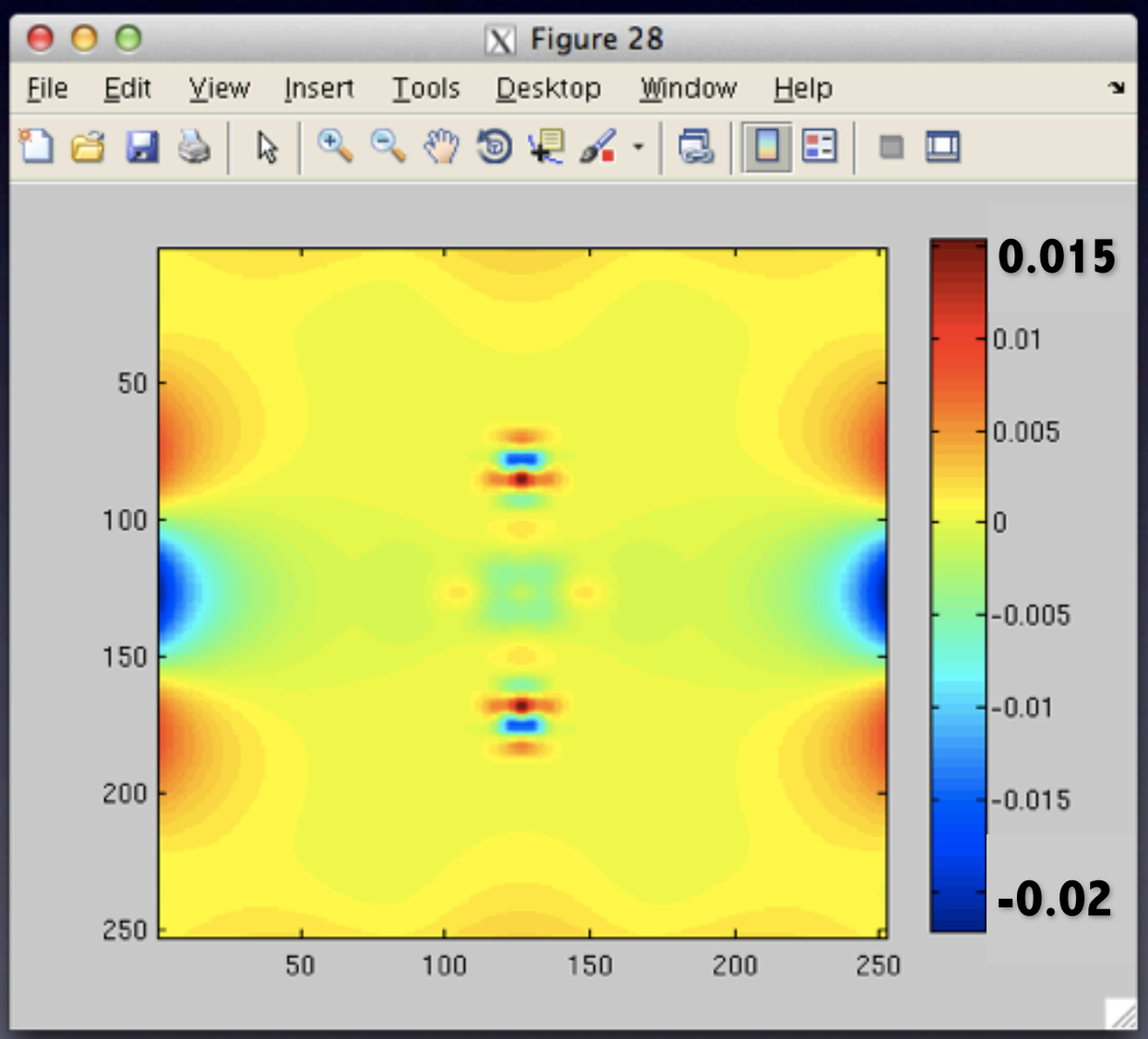


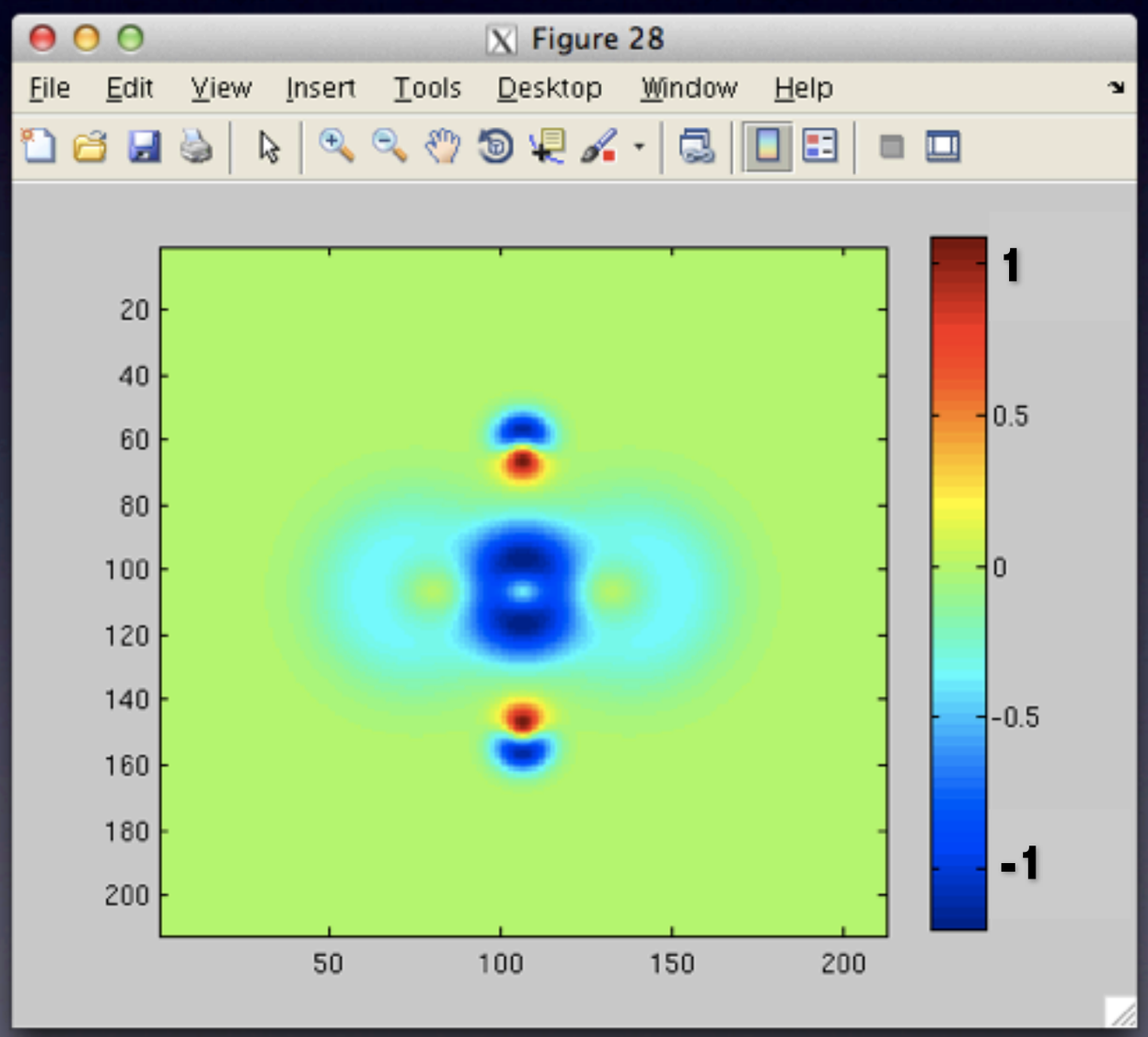
Now:

$$\frac{\max(|\varepsilon_{\text{FFT}}|)}{\max(|\mathbf{F}_{\text{analy}}|)} \sim 2\cdot 10^{-5}$$

Multipole Correction v.s. Green's Function

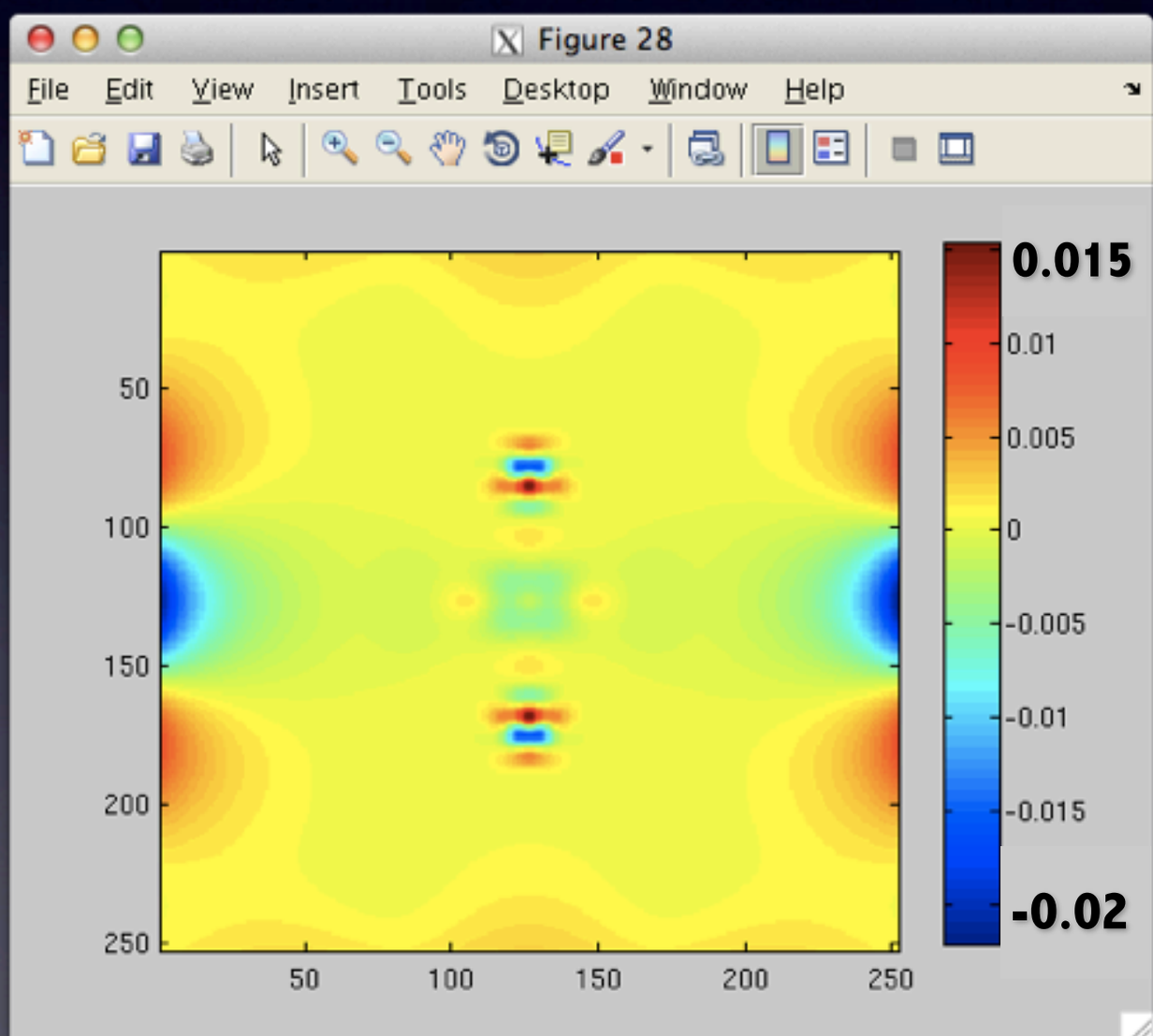
$$\varepsilon_{\mathrm{FFT}} = \left|\mathbf{F}_{\mathrm{FFT}}\right| - \left|\mathbf{F}_{\mathrm{analy}}\right|$$

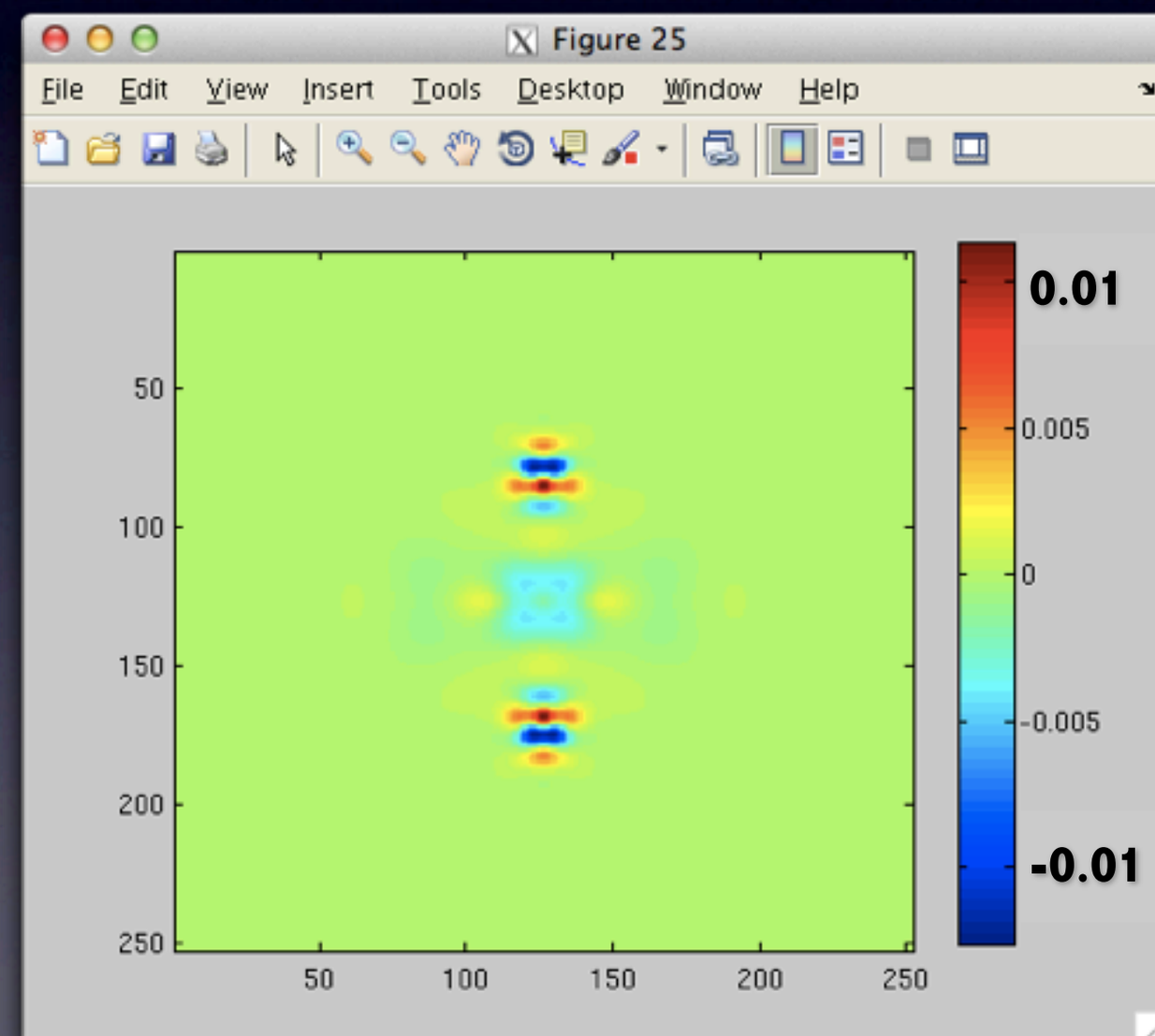




Multipole Correction v.s. Green's Function

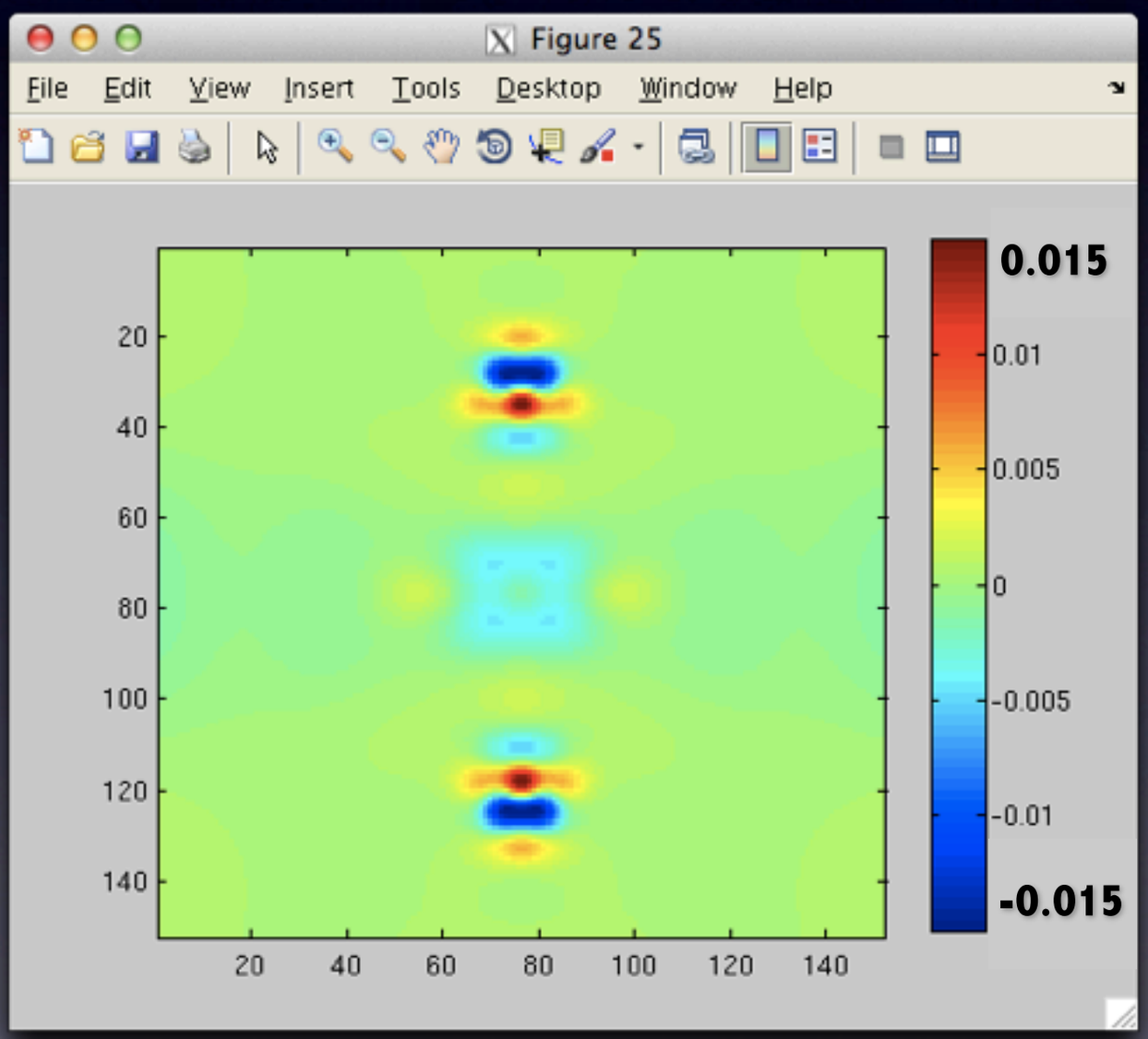
$$\varepsilon_{\mathrm{FFT}} = \left|\mathbf{F}_{\mathrm{FFT}}\right| - \left|\mathbf{F}_{\mathrm{analy}}\right|$$

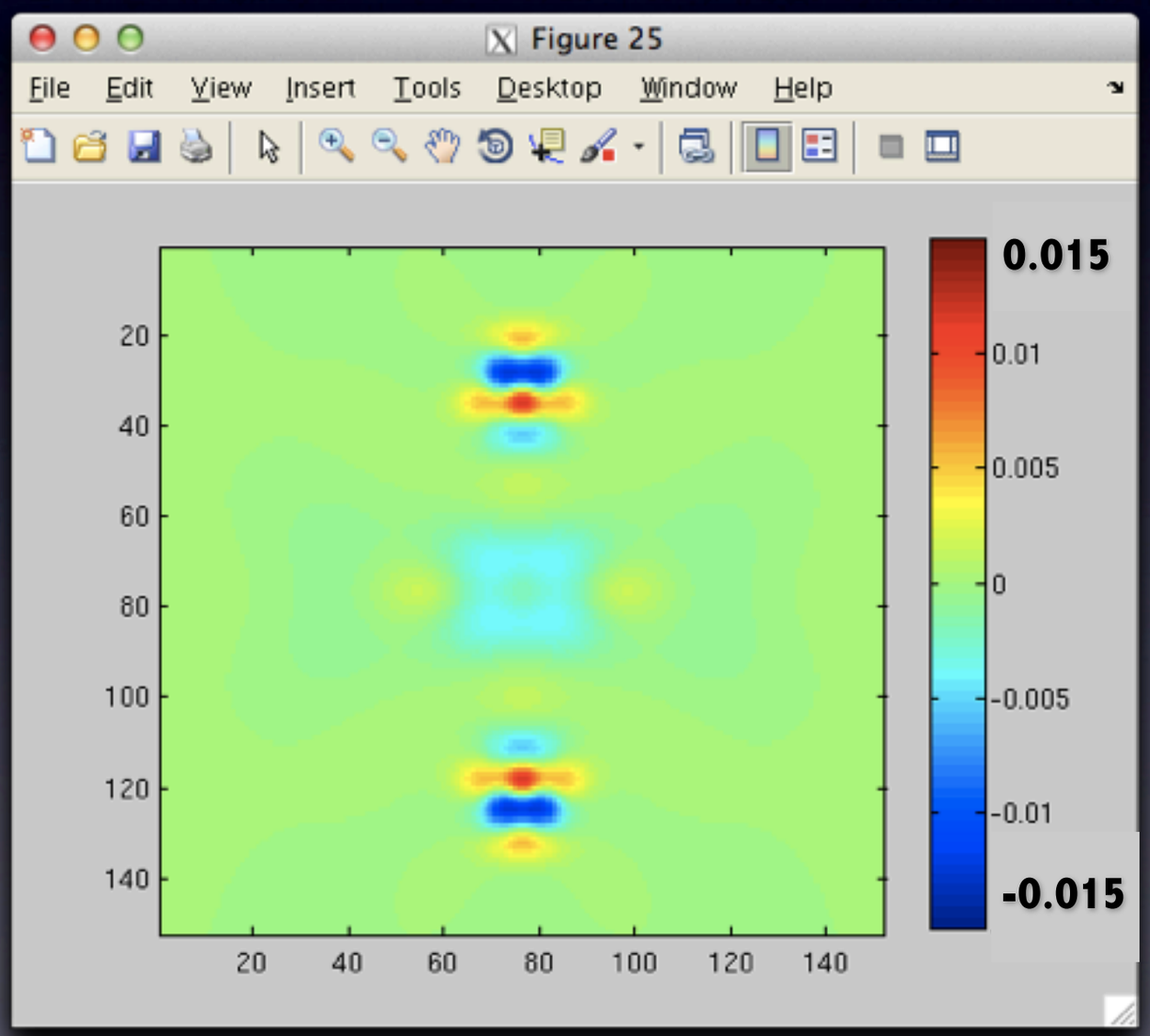




Multipole Correction v.s. Green's Function

$$\varepsilon_{\mathrm{FFT}} = \left|\mathbf{F}_{\mathrm{FFT}}\right| - \left|\mathbf{F}_{\mathrm{analy}}\right|$$





Multipole Correction v.s. Green's Function

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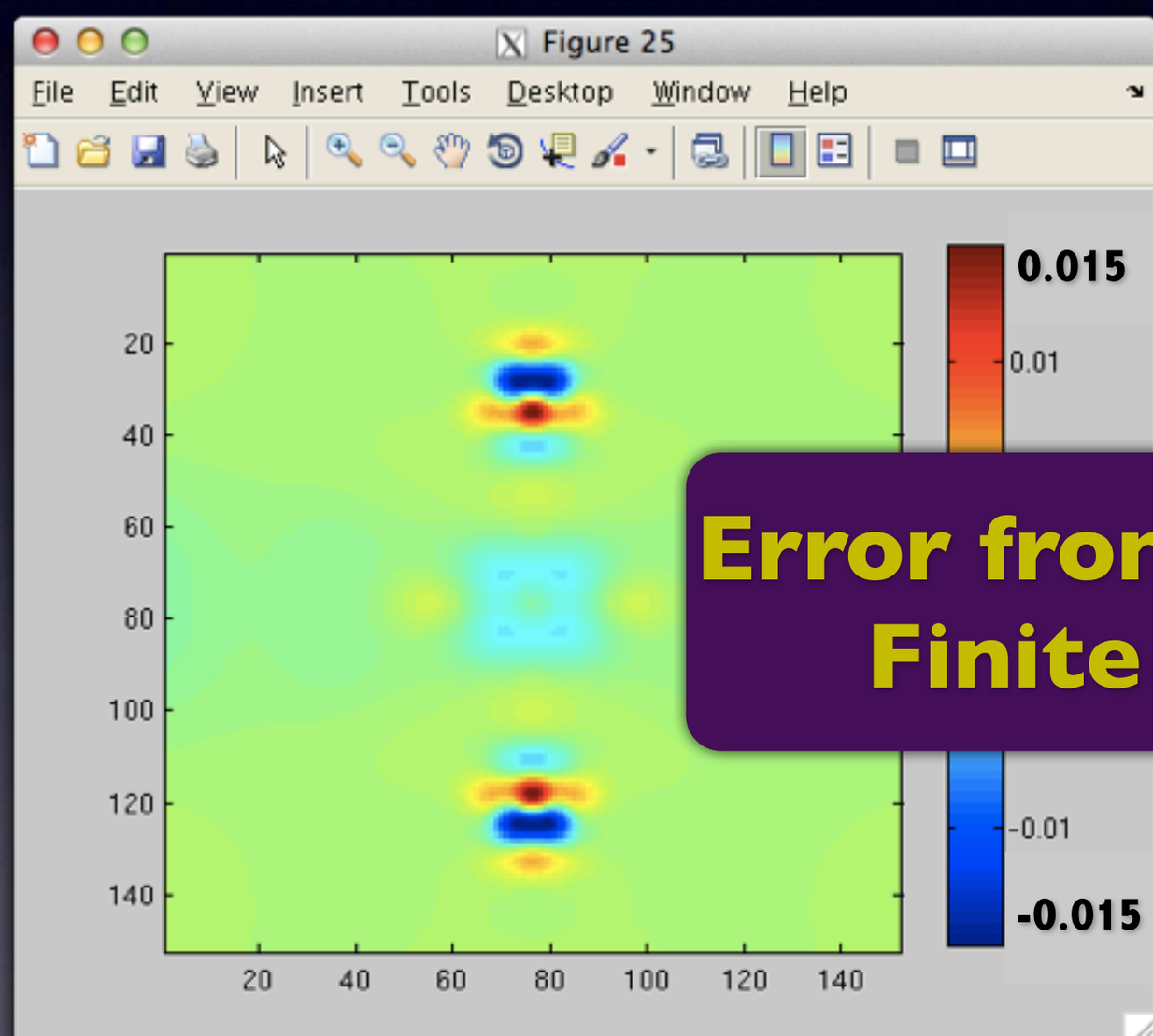
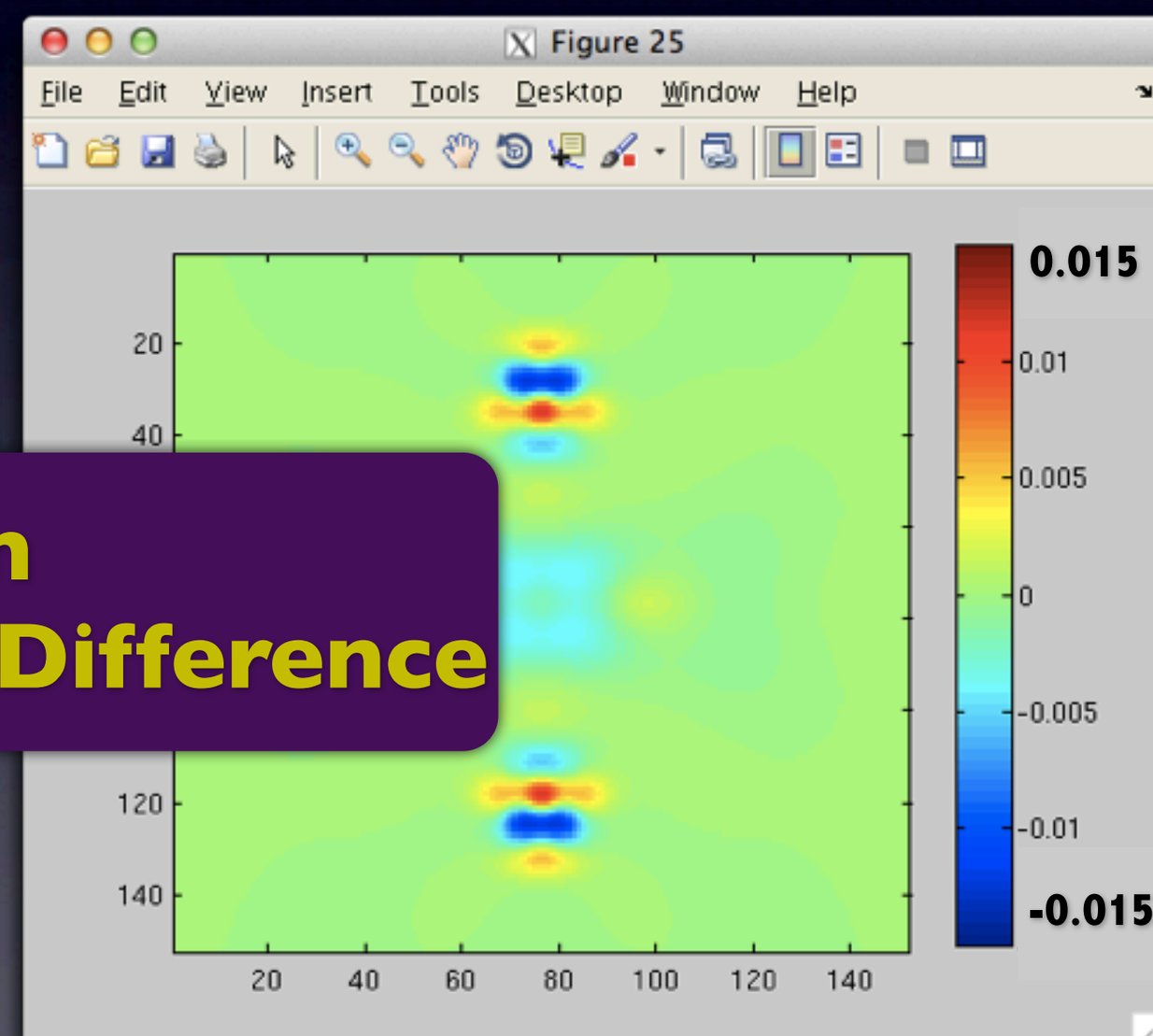




Error from Finite Difference

FFT Force

- Green's Function

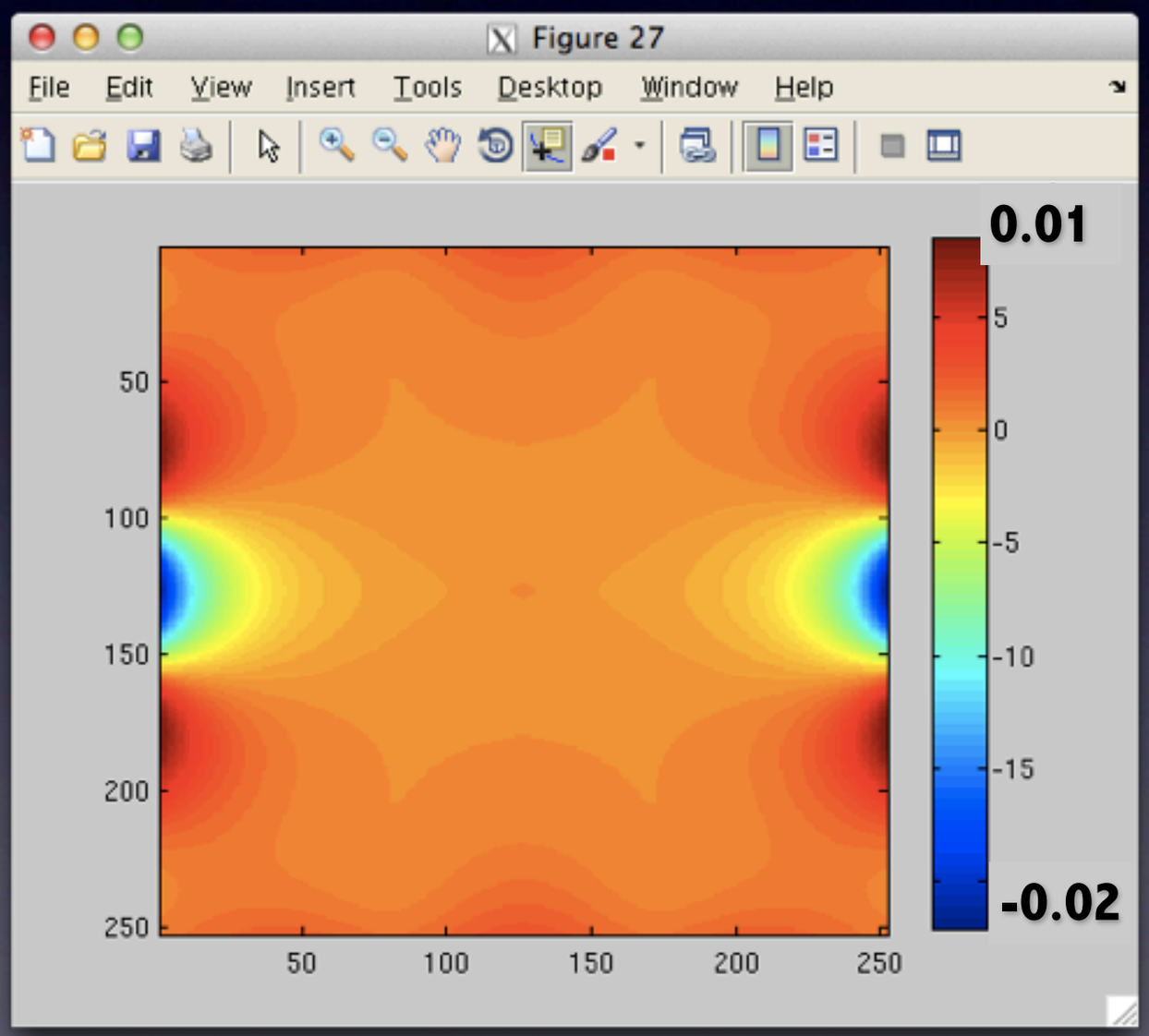
$$\mathbf{F}(\mathbf{x}) = \nabla\phi(\mathbf{x}) = \int \left[\nabla G(\mathbf{x}-\mathbf{x}')\right]\rho(\mathbf{x}')d^3x'$$

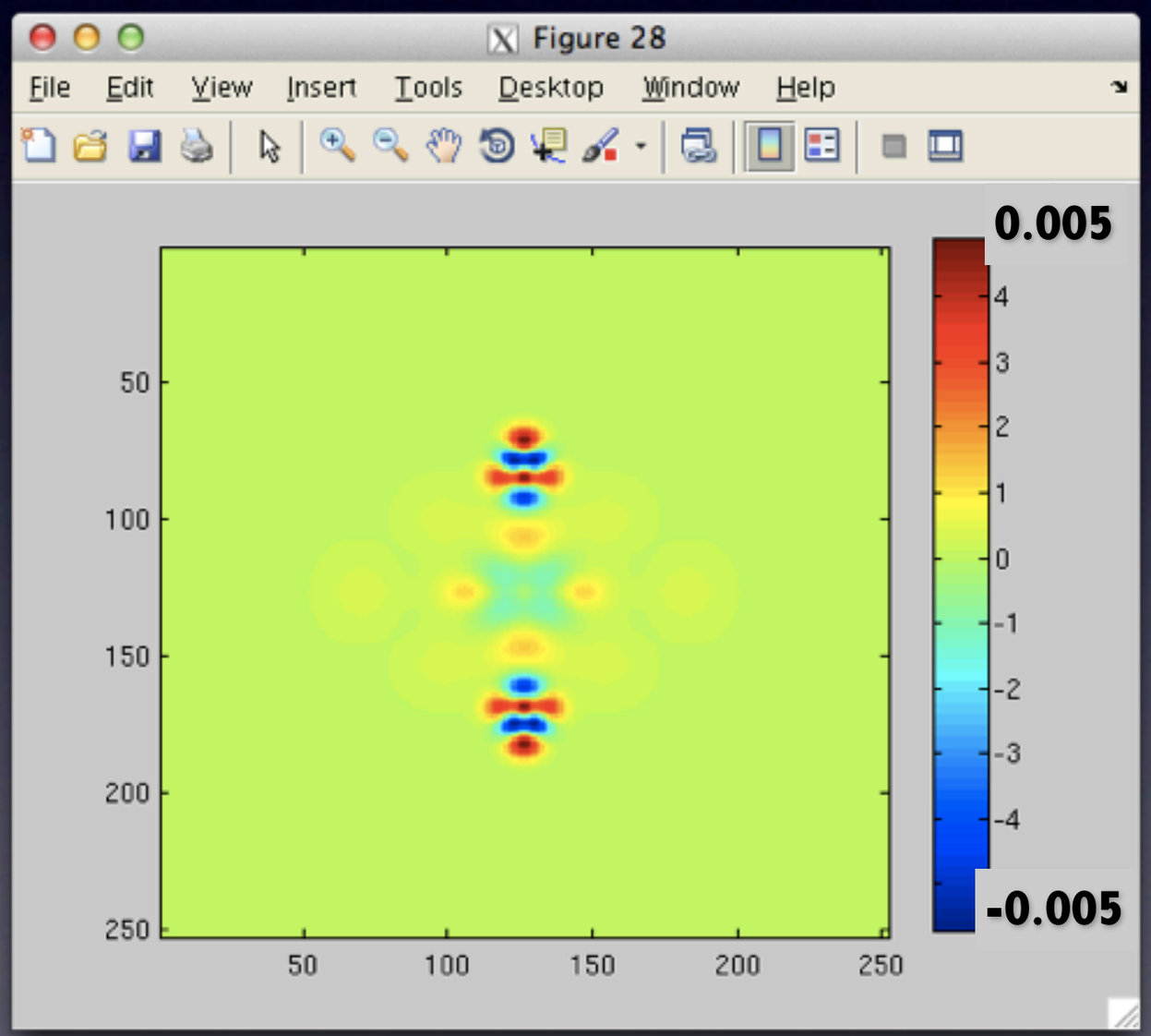
- Multipole Correction

$$\mathbf{F} = \mathbf{F}^{\mathrm{FFT}} - \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left(\mathbf{F}_{lm}^{\mathrm{FFT}} - \mathbf{F}_{lm}^{\mathrm{analy}}\right)$$

Multipole Correction v.s. Green's Function

$$\varepsilon_{\mathrm{FFT}} = \left|\mathbf{F}_{\mathrm{FFT}}\right| - \left|\mathbf{F}_{\mathrm{analy}}\right|$$





Multipole Correction v.s. Green's Function

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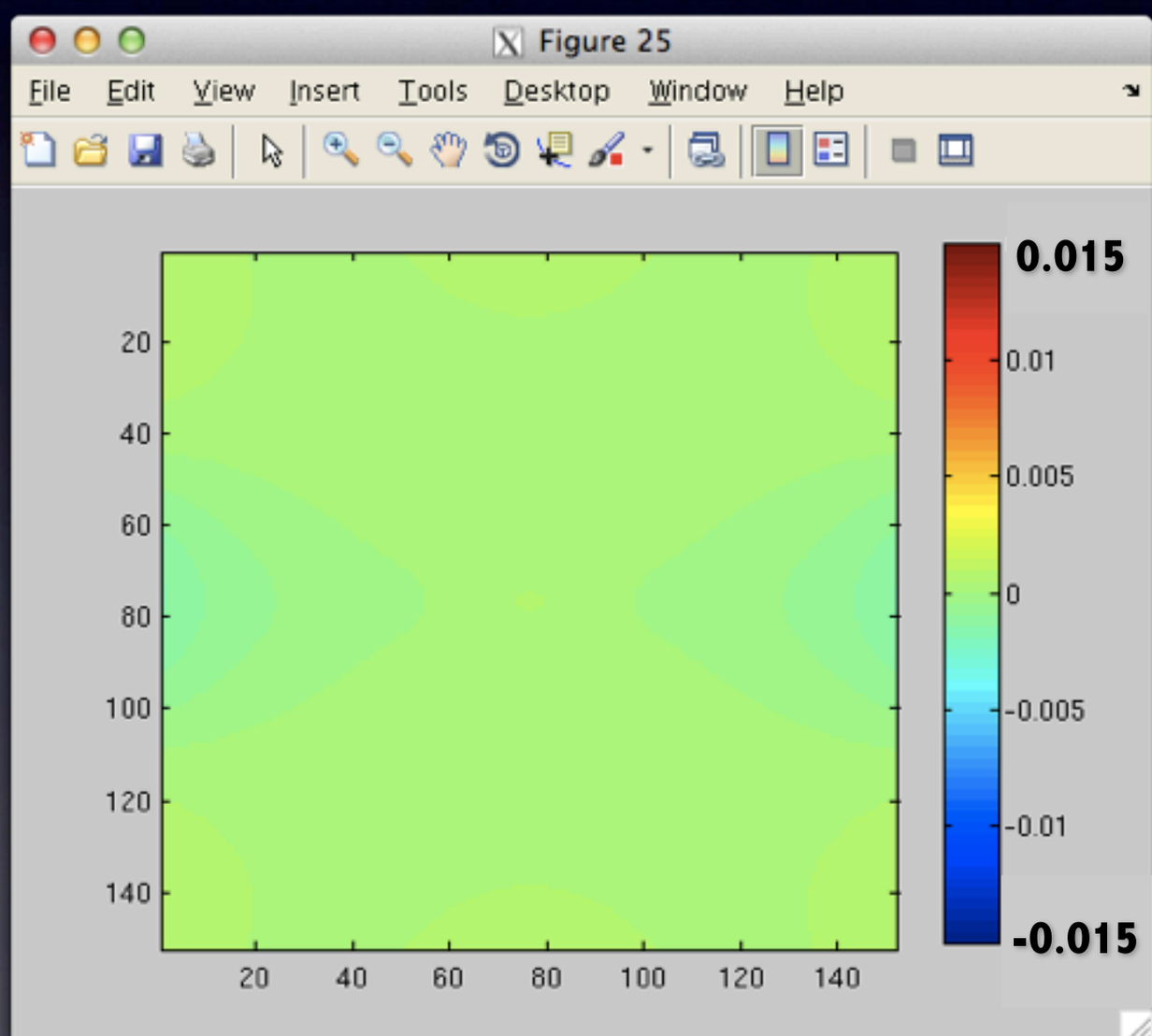

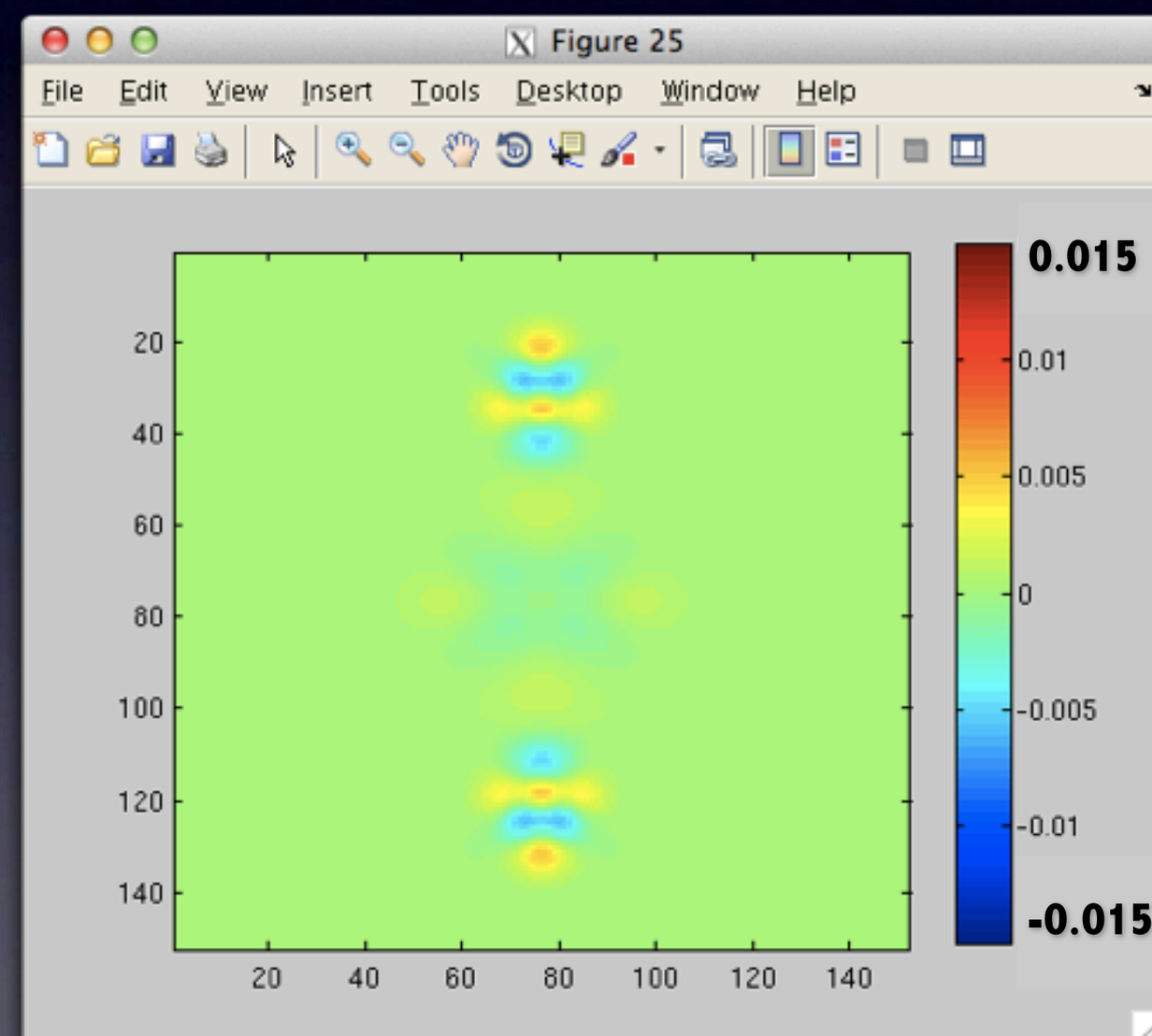

Multipole Correction v.s. Green's Function

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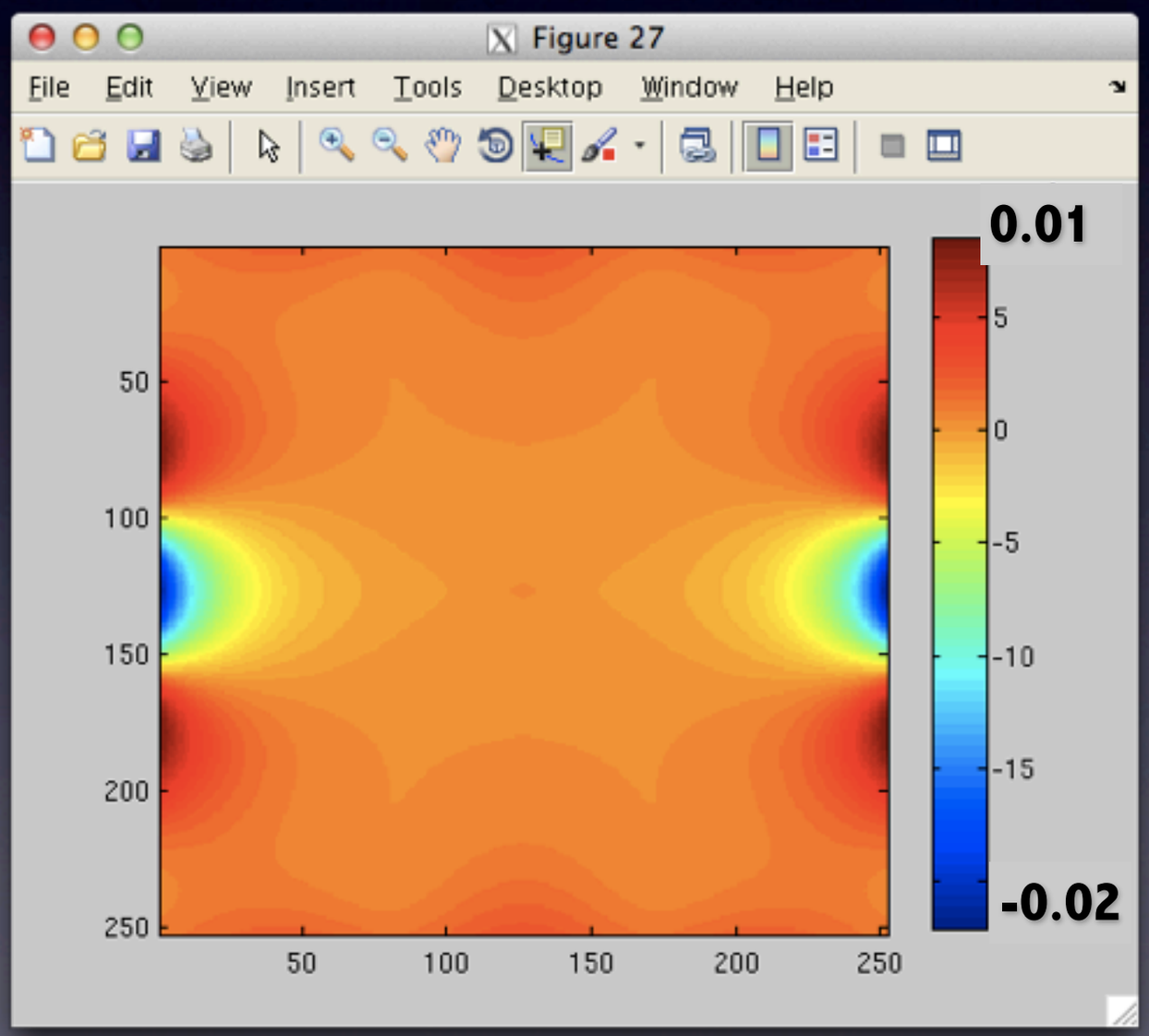
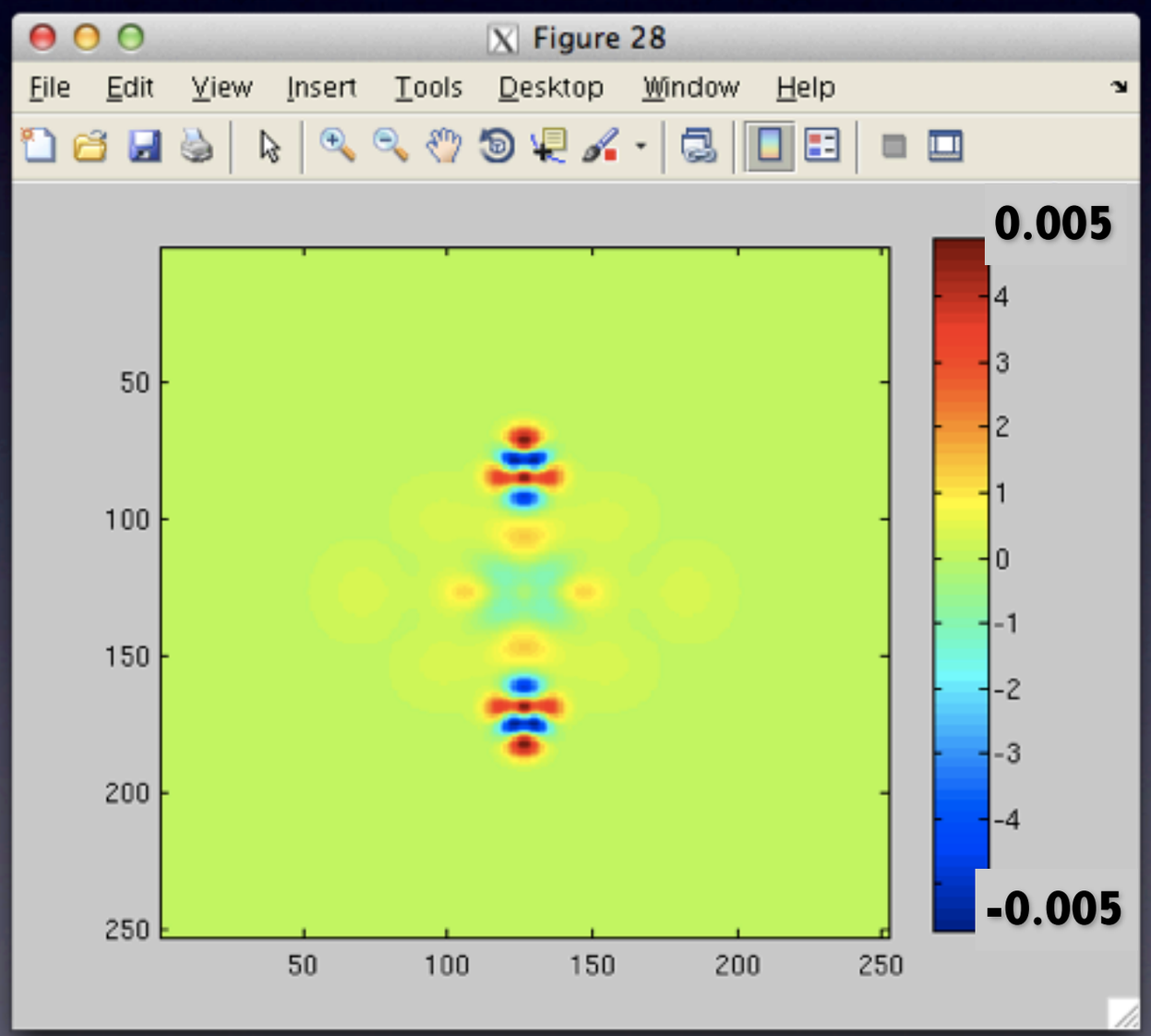




Computation Efficiency

Speed ratio

$$= \frac{T_{Green}}{T_{Multipole}}$$

T_{Green} : running time with Green's func.

$T_{Multipole}$: running time with Multipole corr.

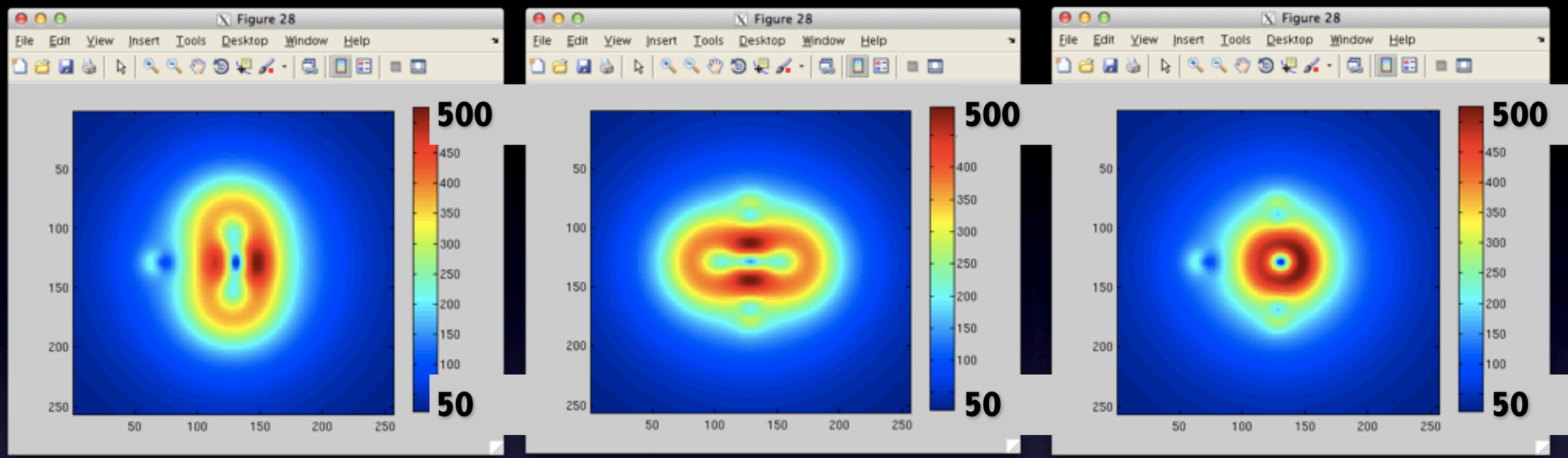
	64^3	128^3	256^3	512^3
CPU	3.60	3.63	3.60	3.53

Pros & Cons

Multipole Correction	Green's Function
Error free when $\ell \rightarrow \infty$	Singularity number optimizaton
Error is larger at peripheral region	Error is larger at denser region
3.6 times faster	
80% memory usage of Green's function	

Thank you

Error from Multipole Force Corr.



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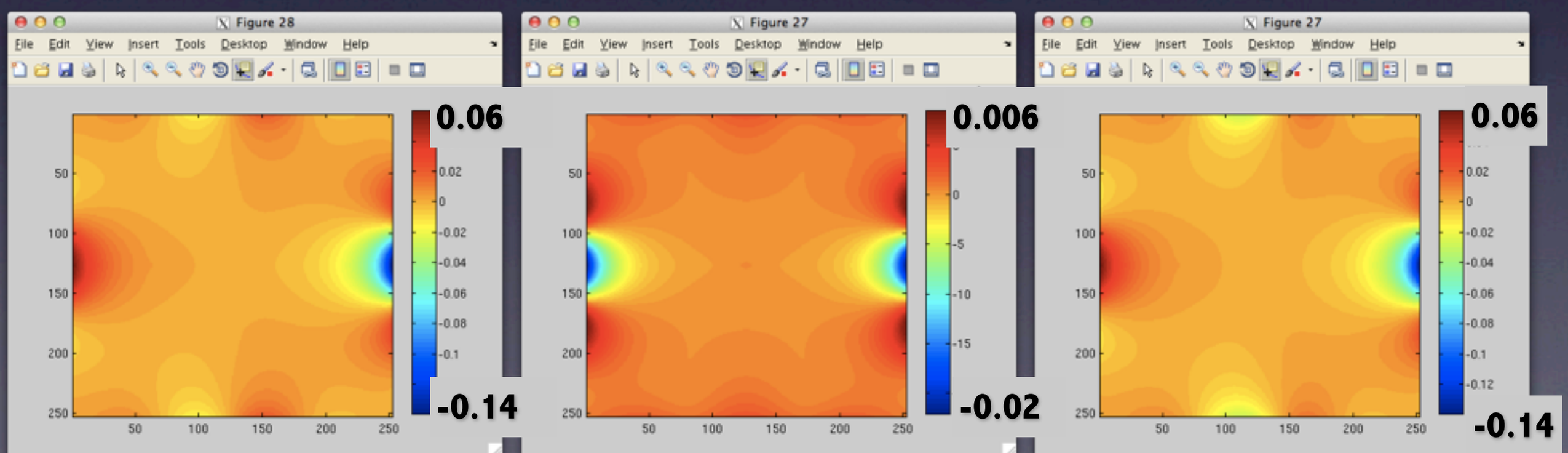
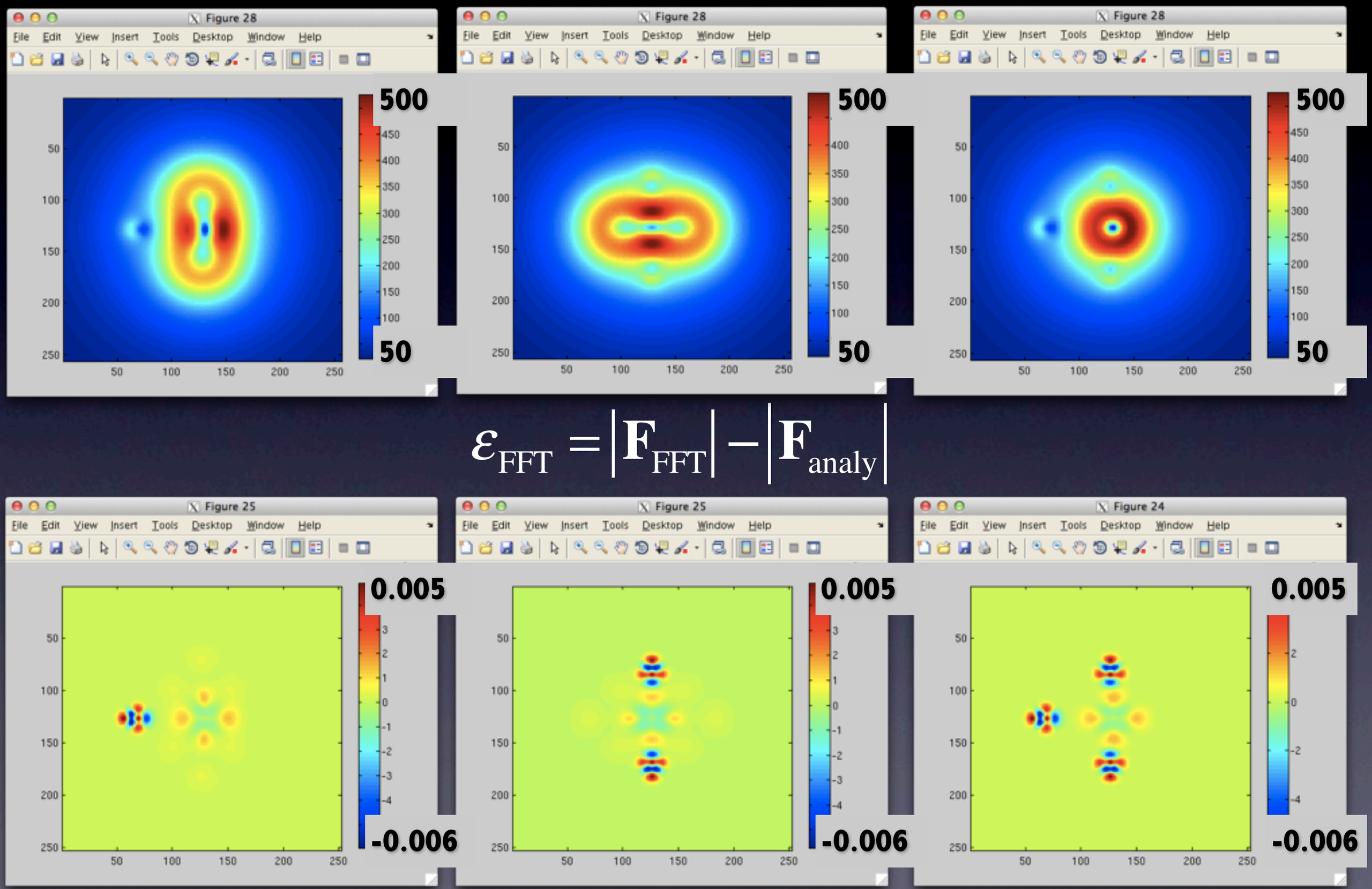


Error from Green's Function Force Corr.



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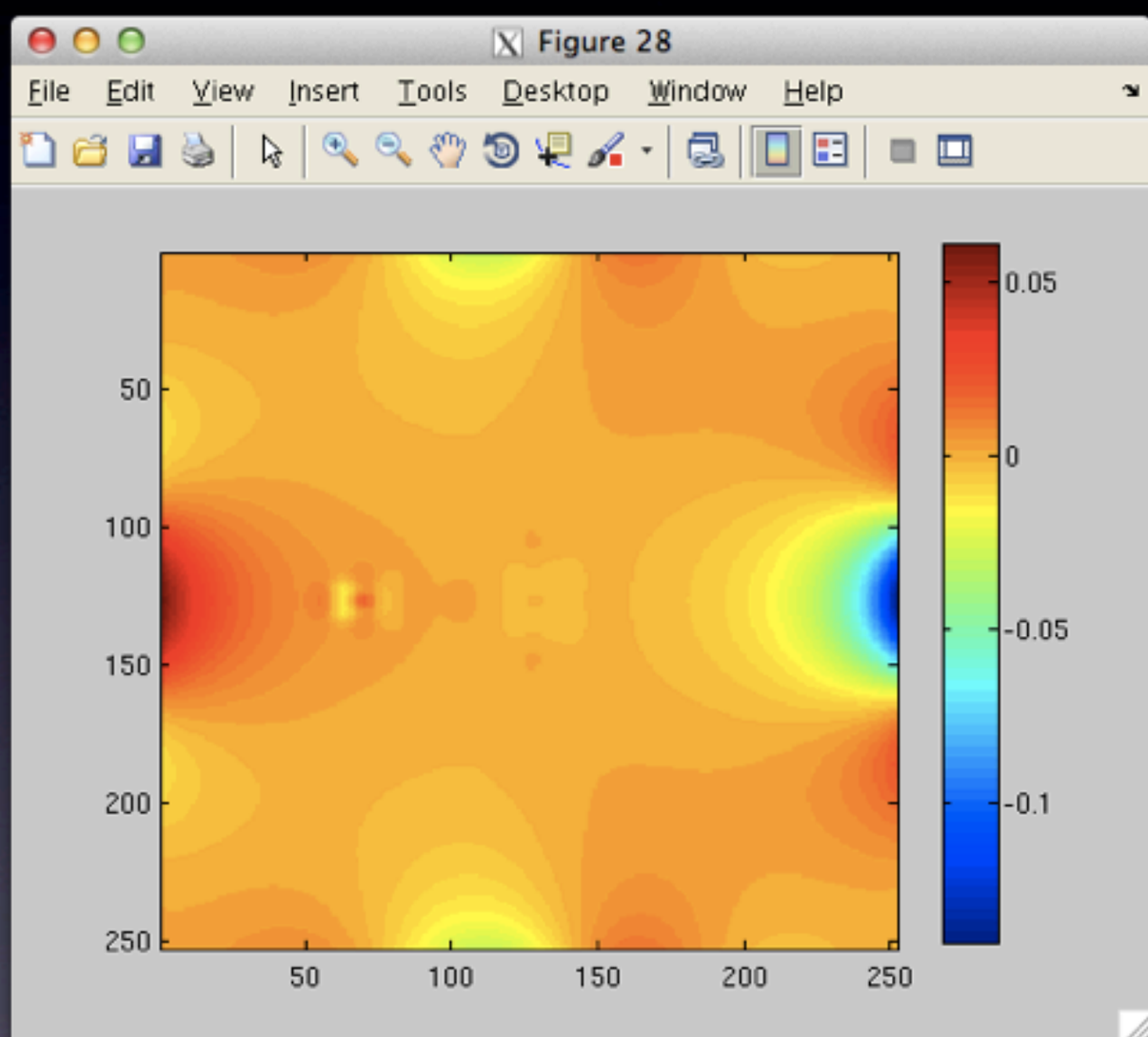
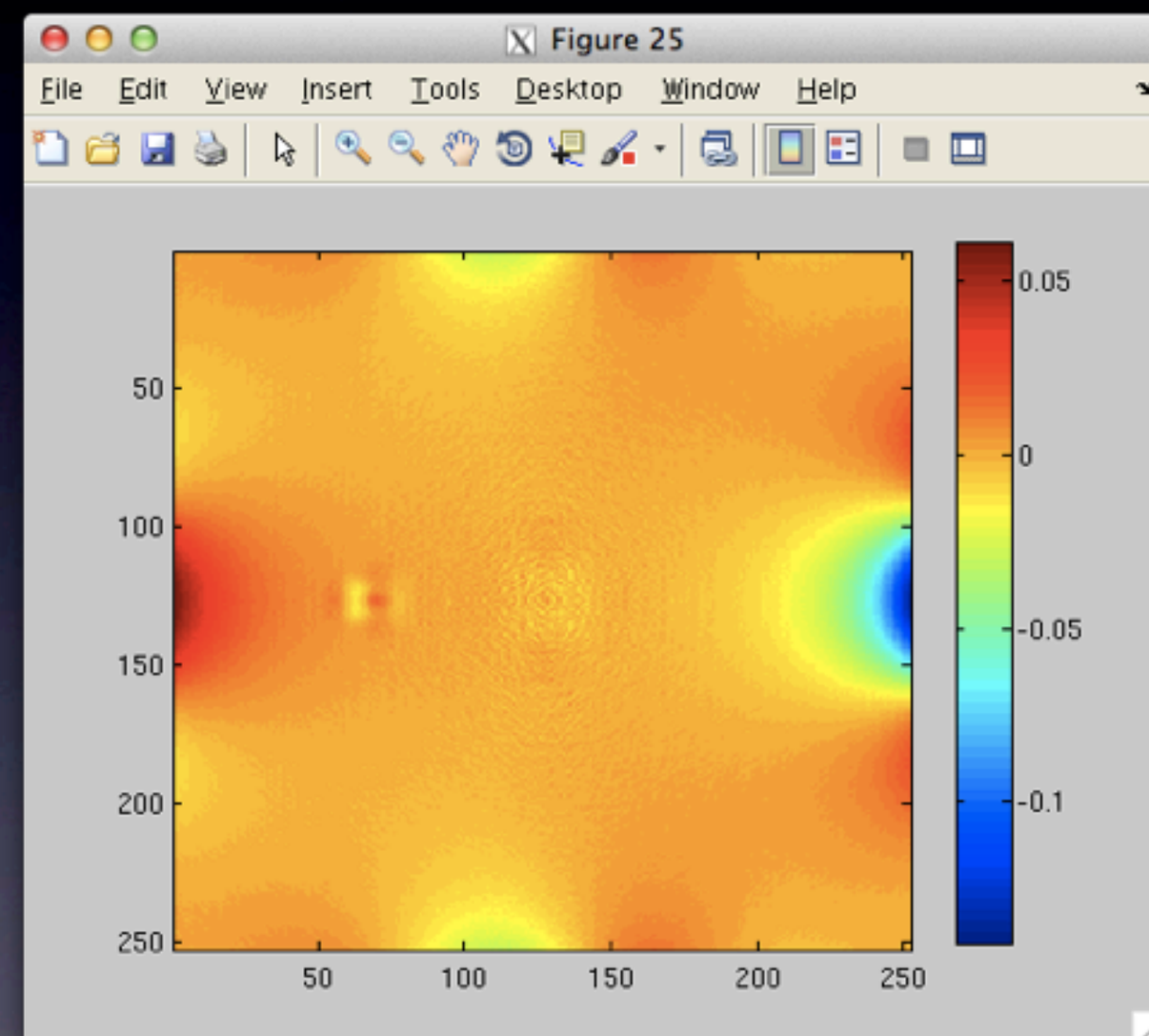
Double and Single Precision

Double and Single Precision





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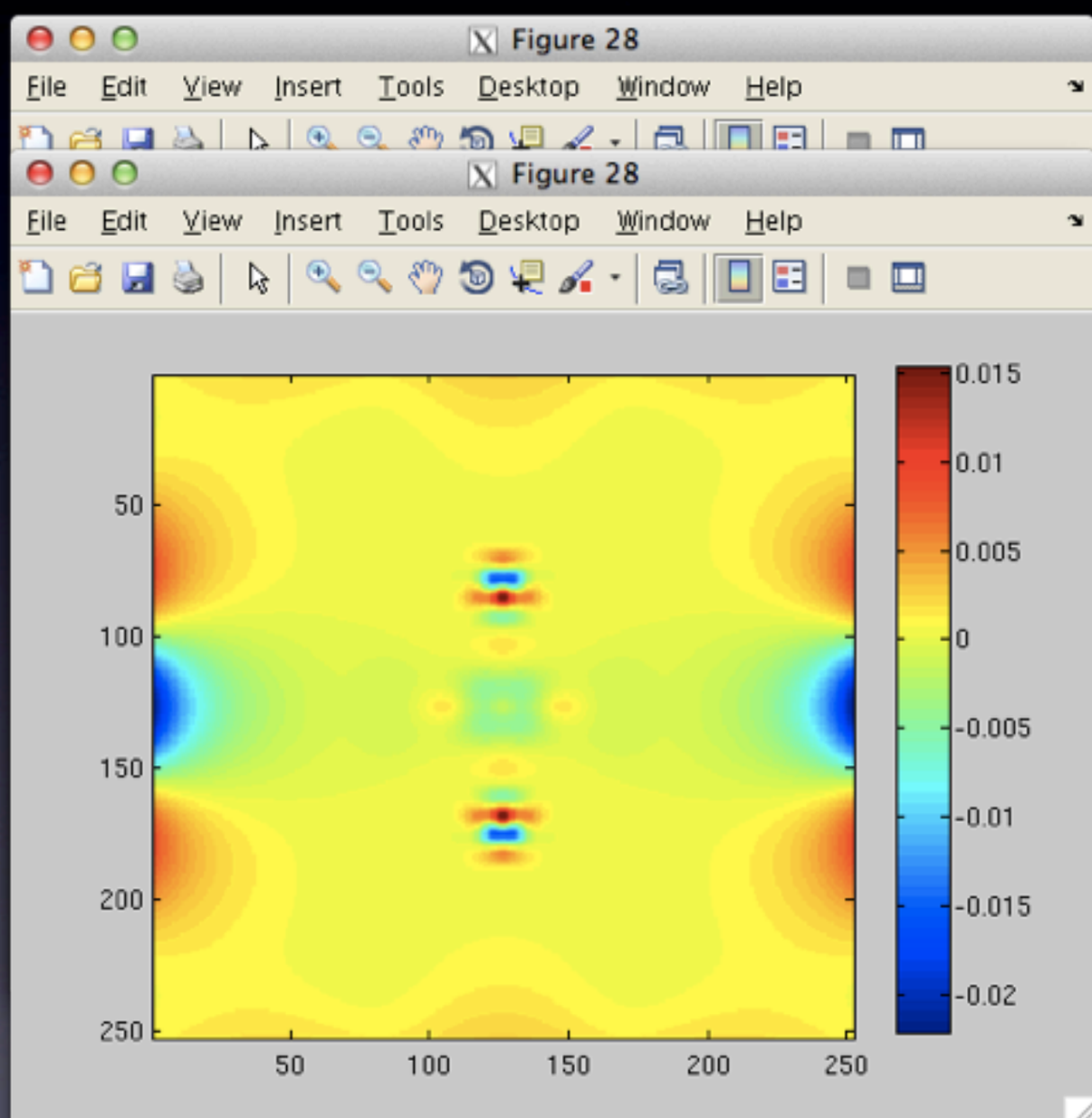

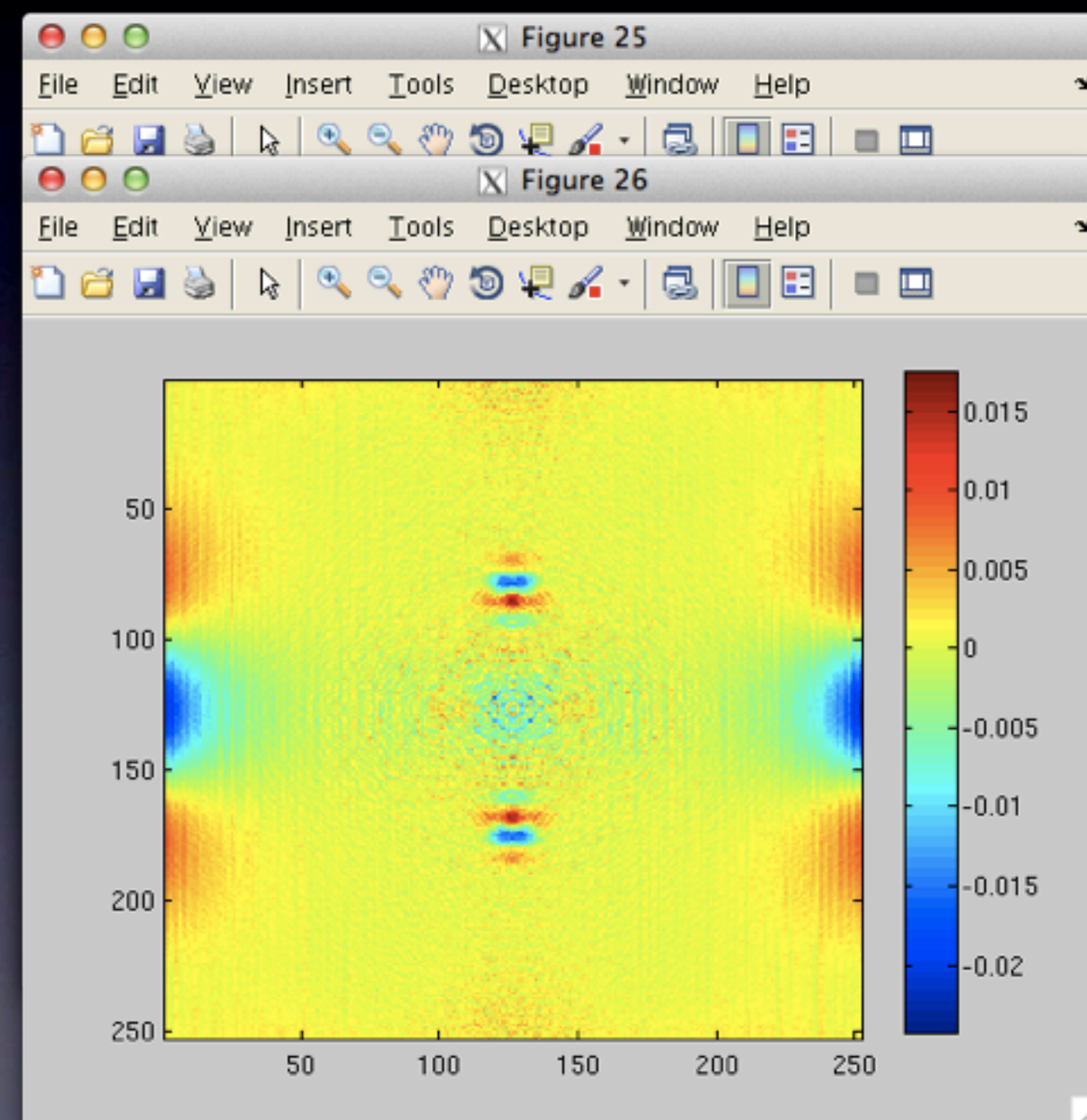

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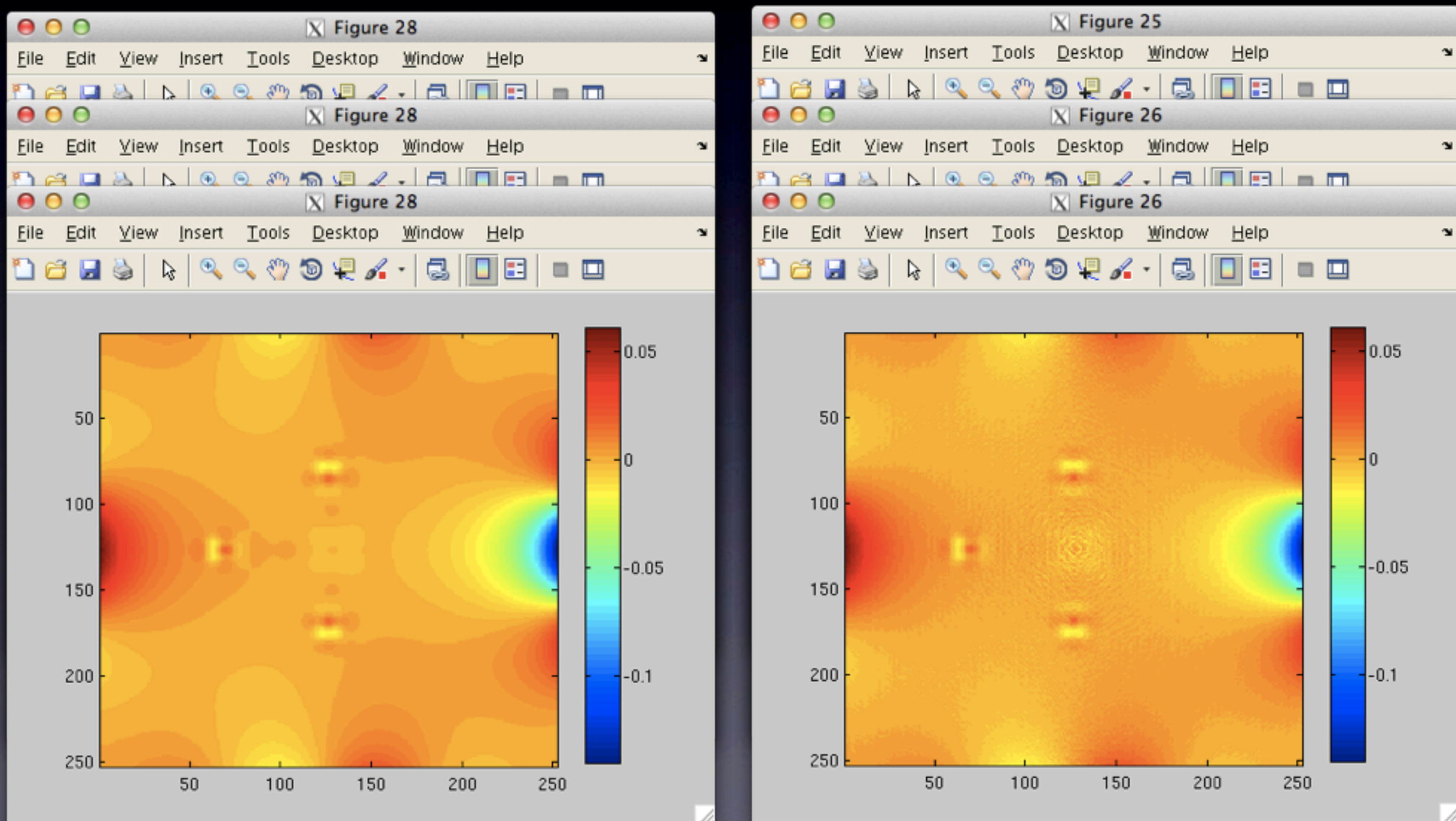
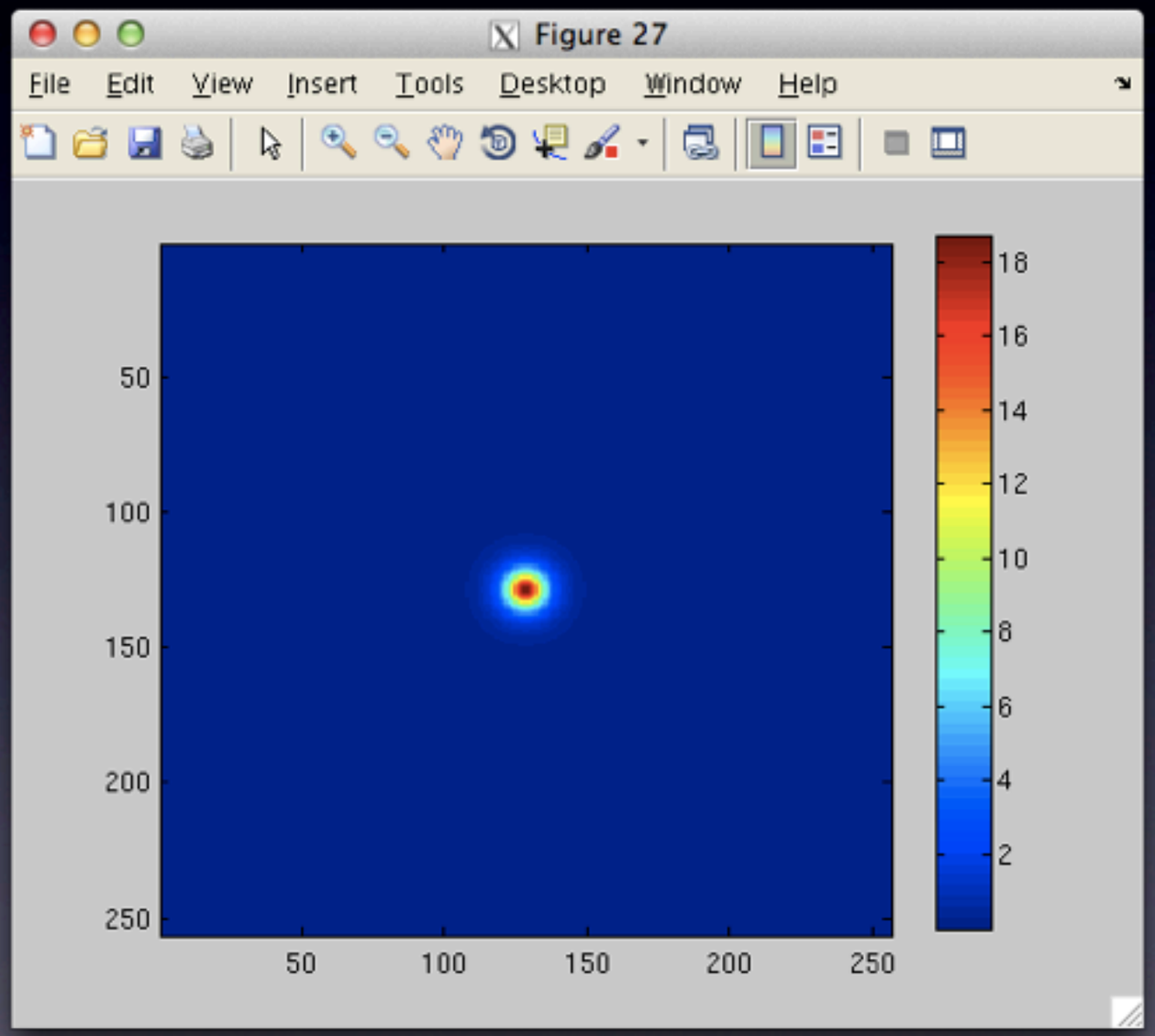


Plummer Model (force corr.)



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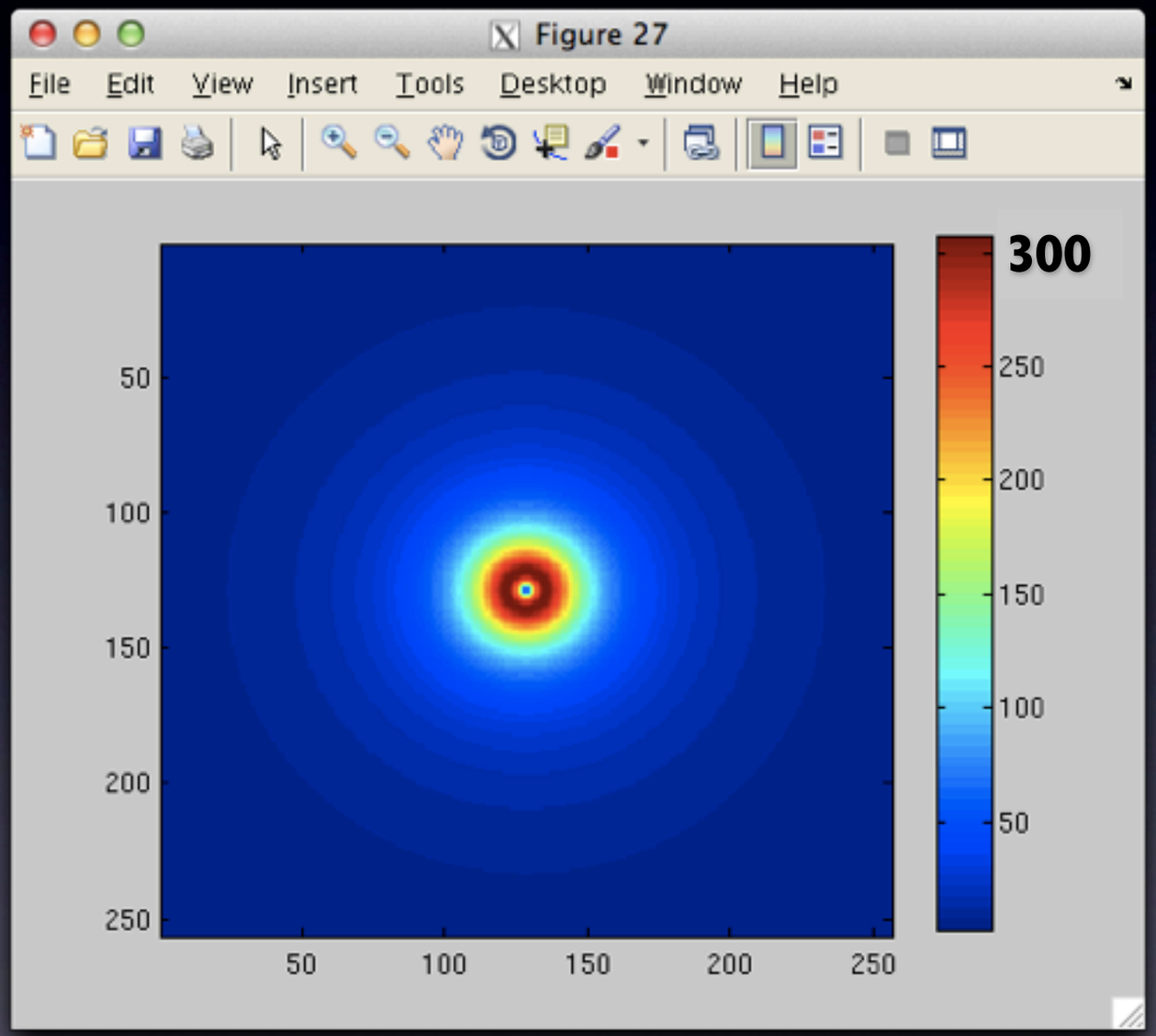

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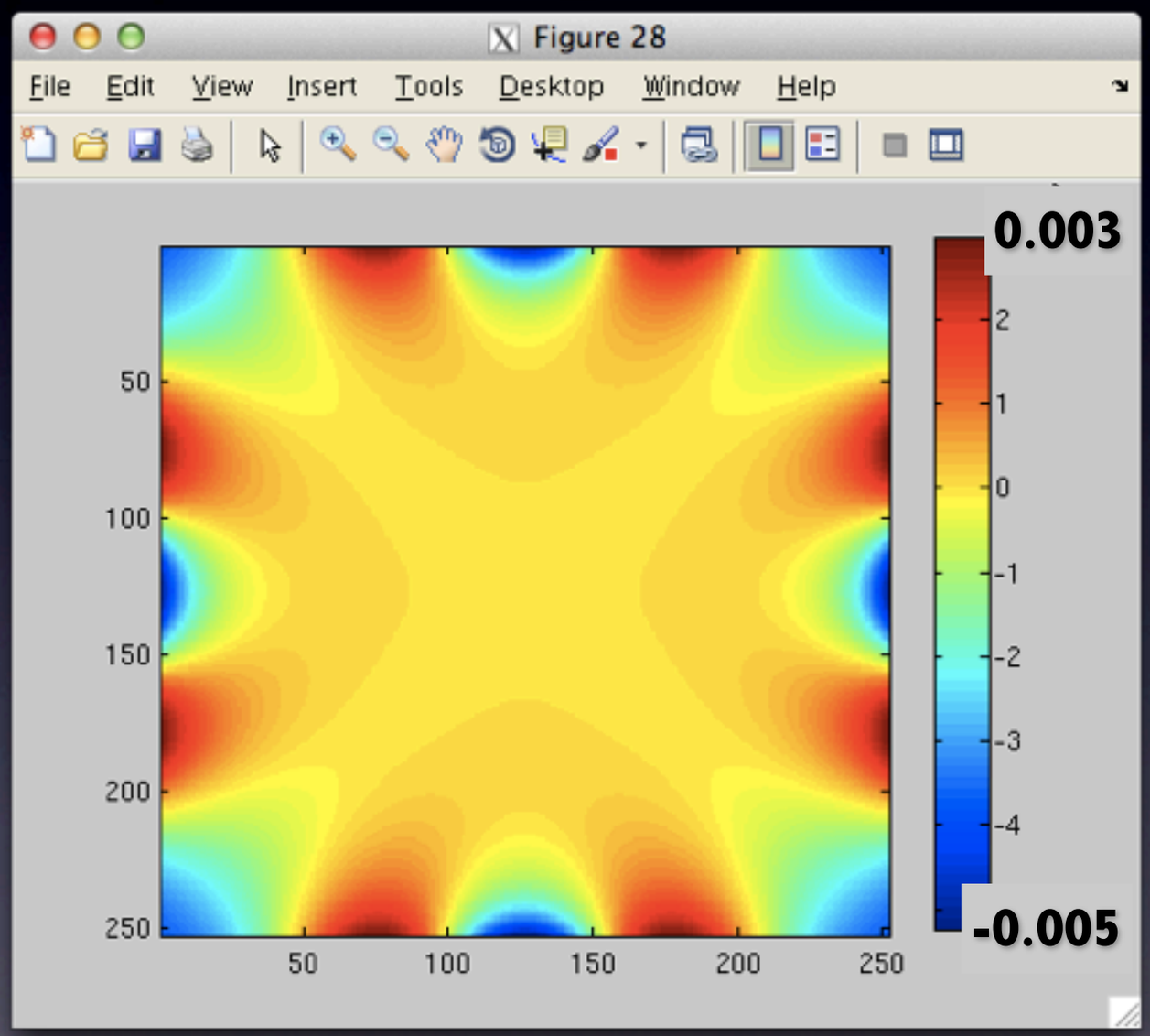

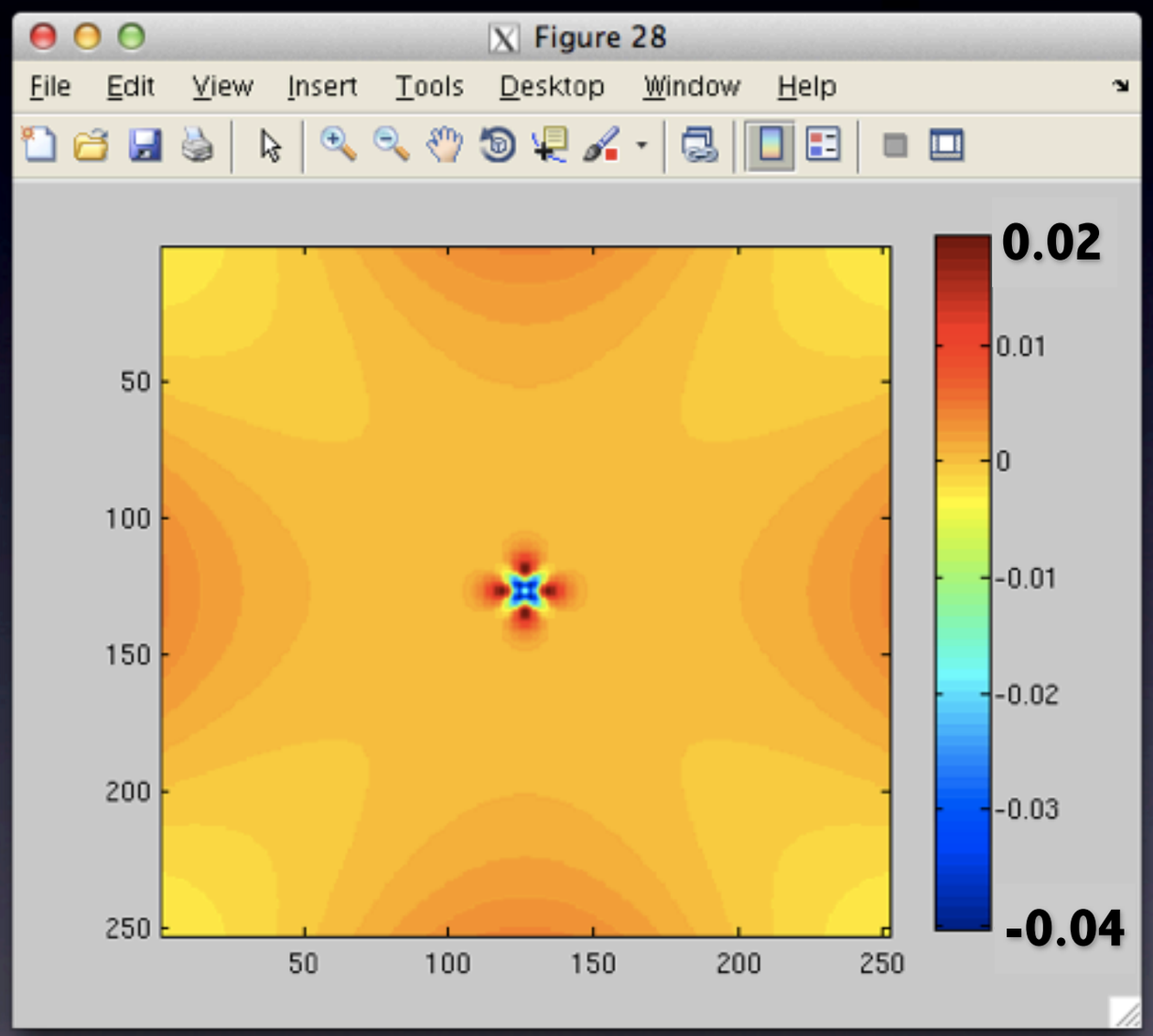

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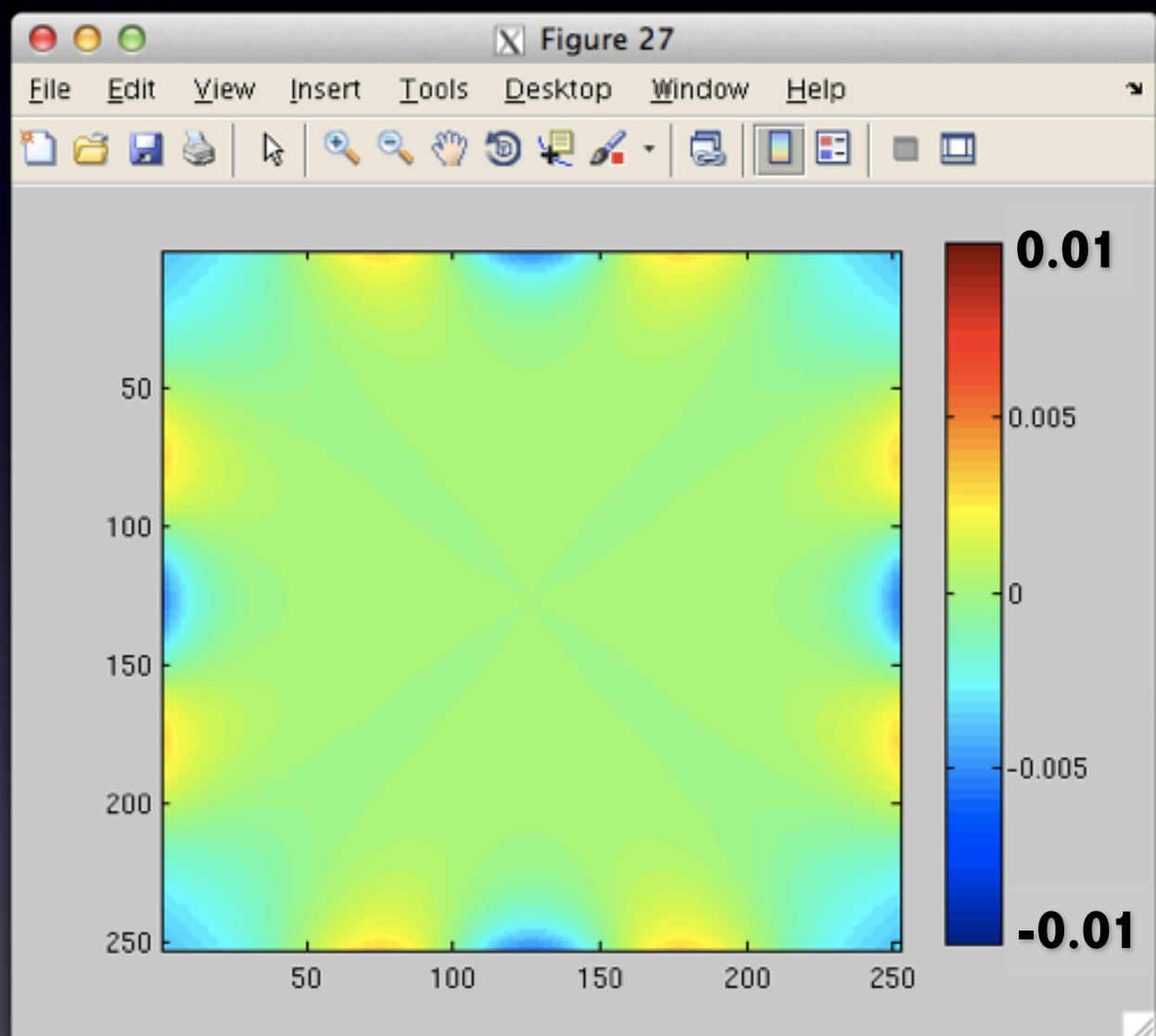
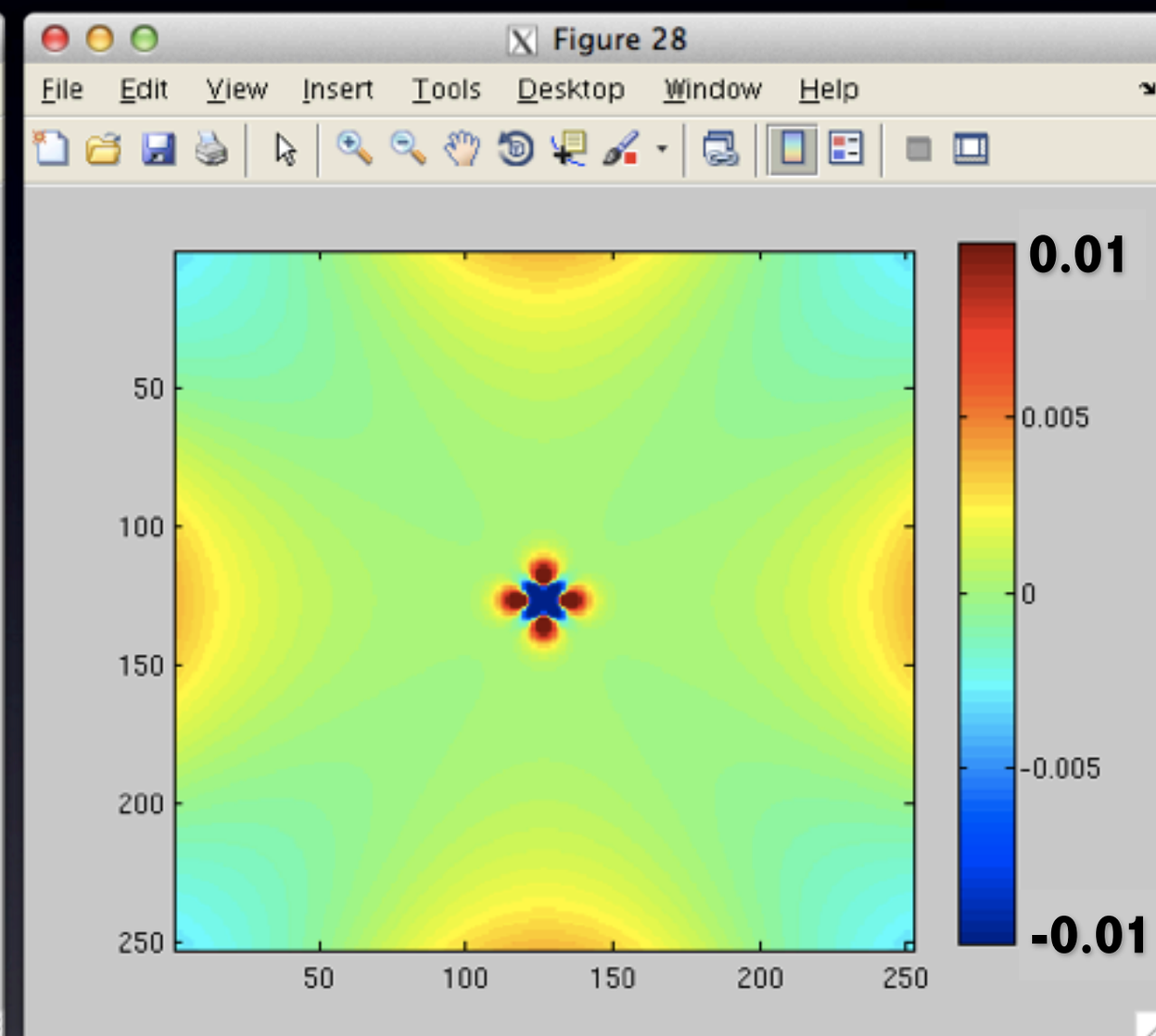
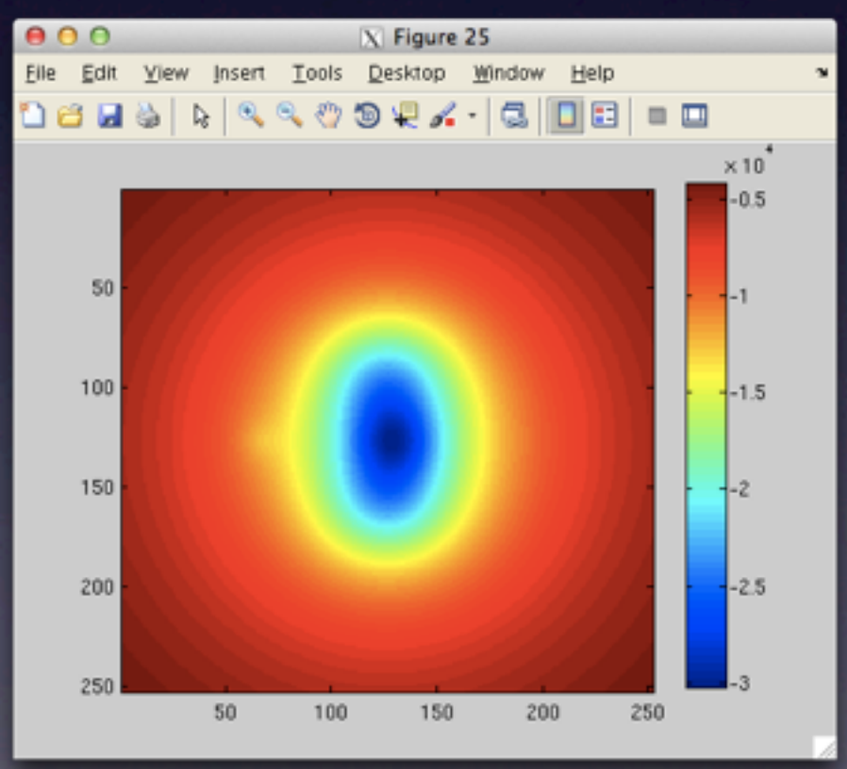


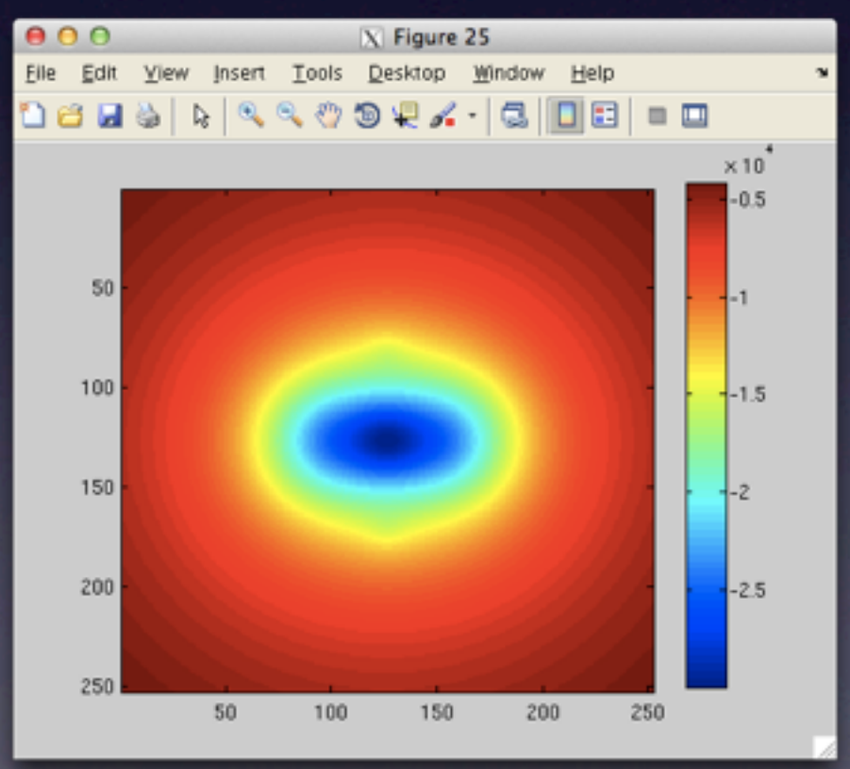


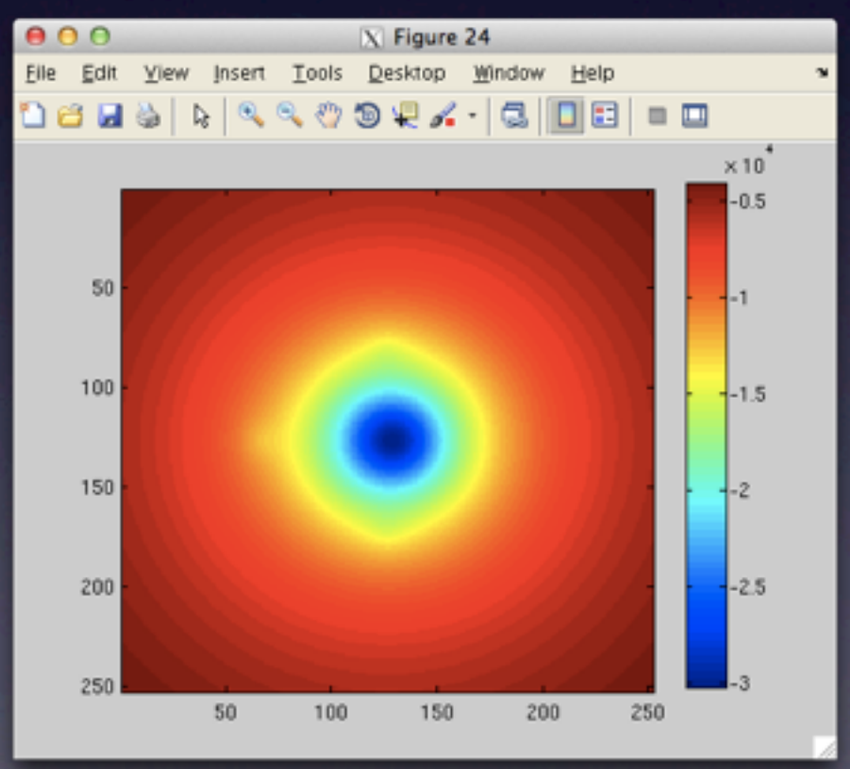
Green's function singularity adaption

Green's function singularity adaption

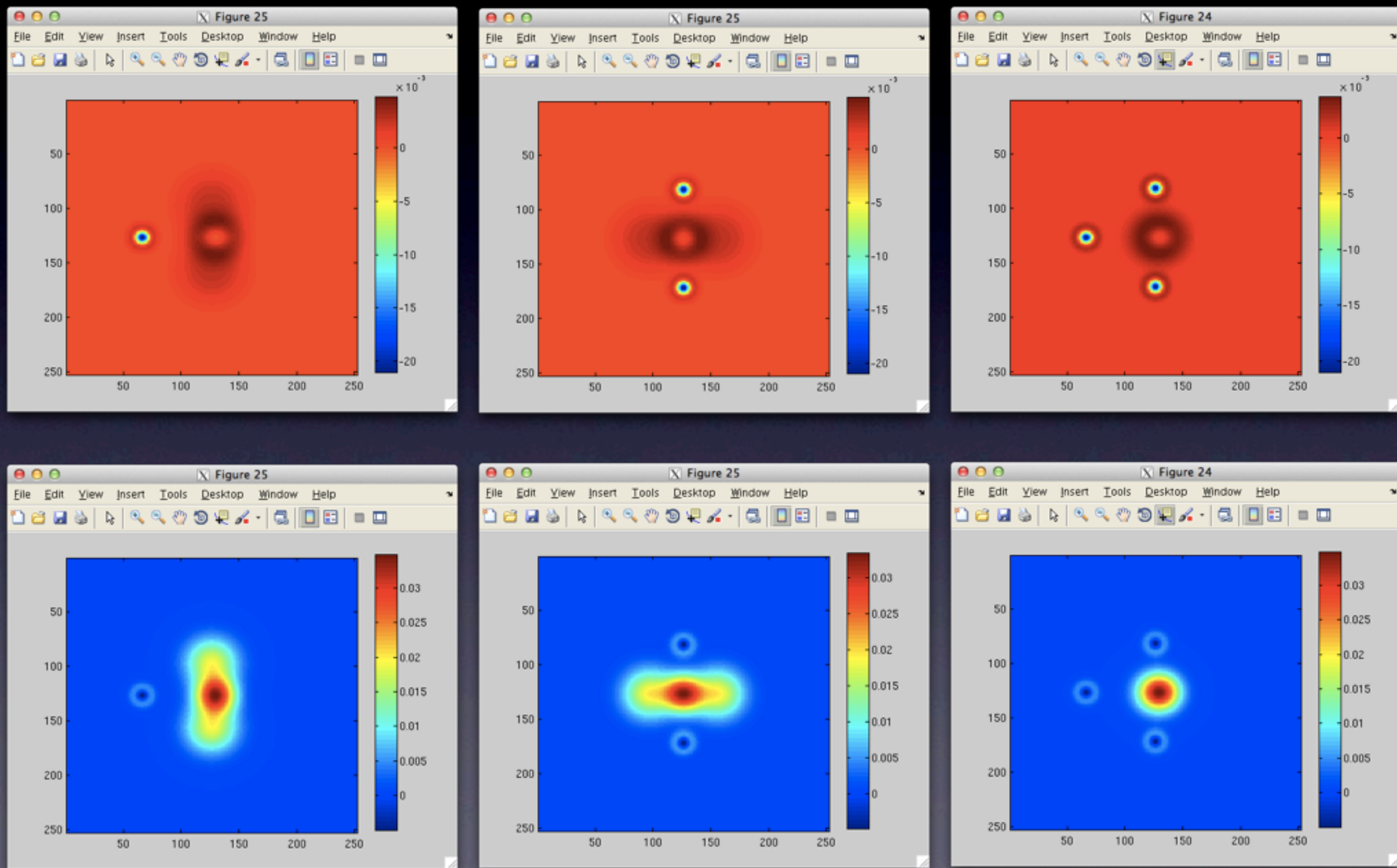
Potential Field





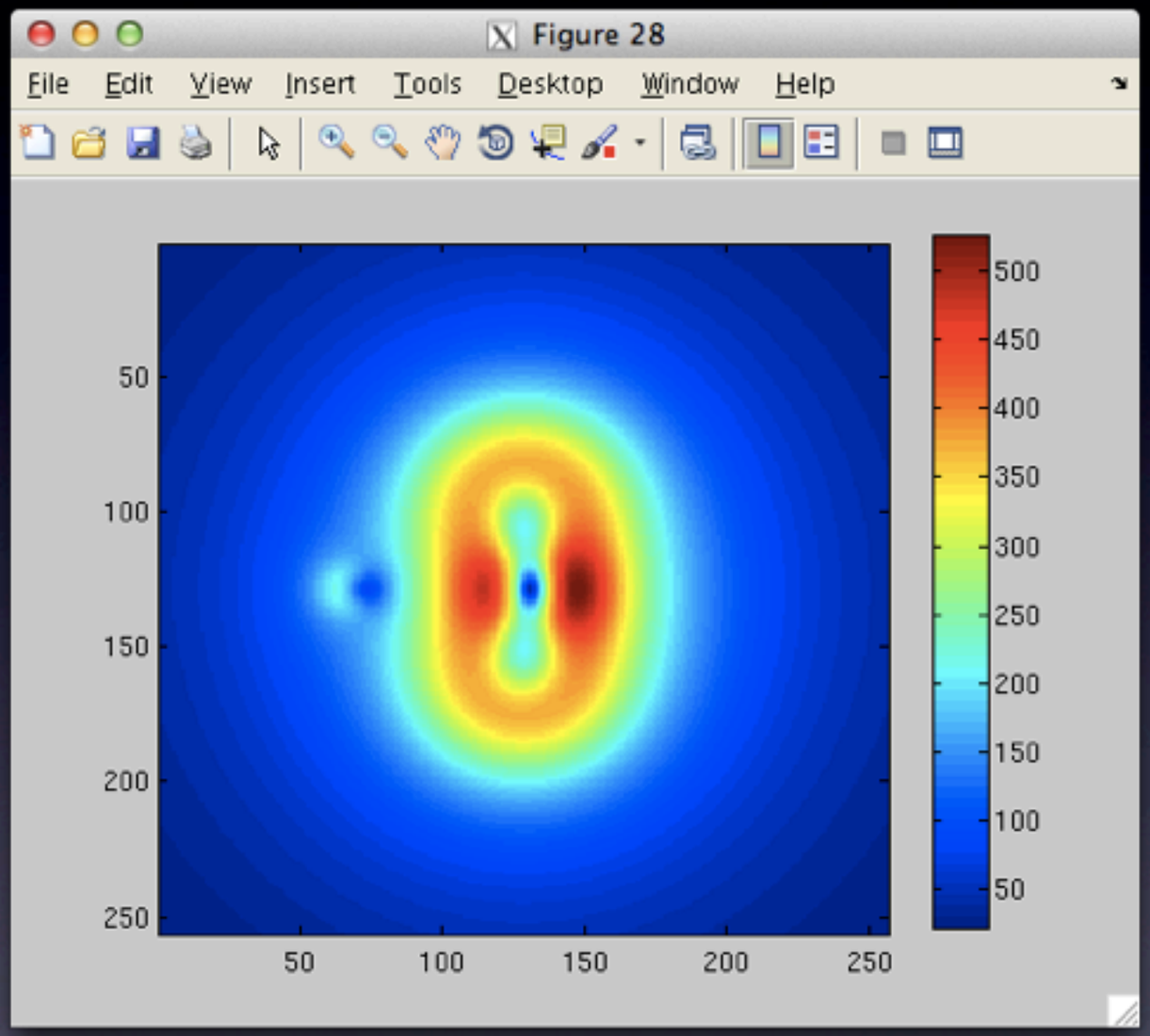


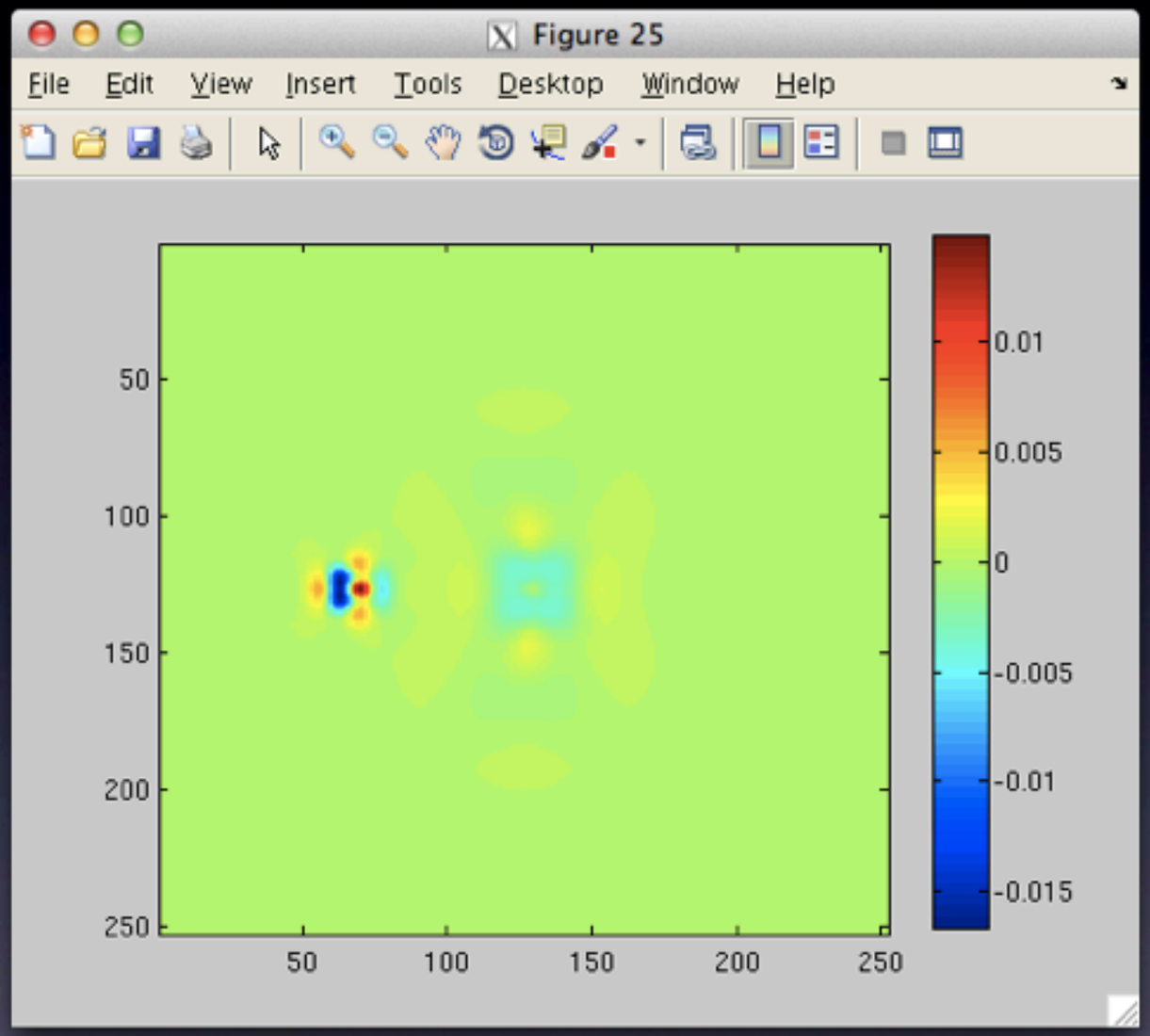
Green's function singularity adaption



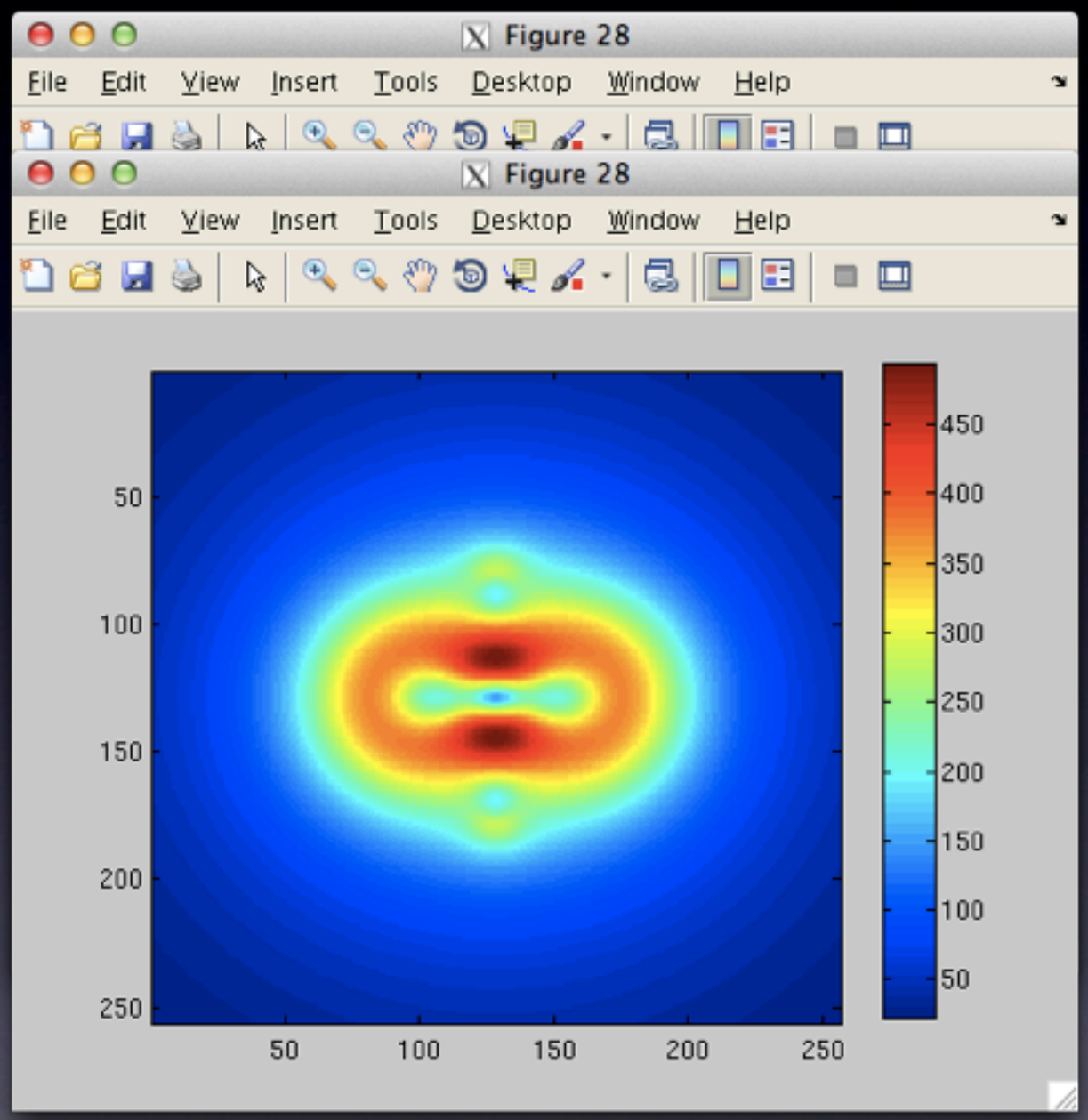
Finite Difference Method

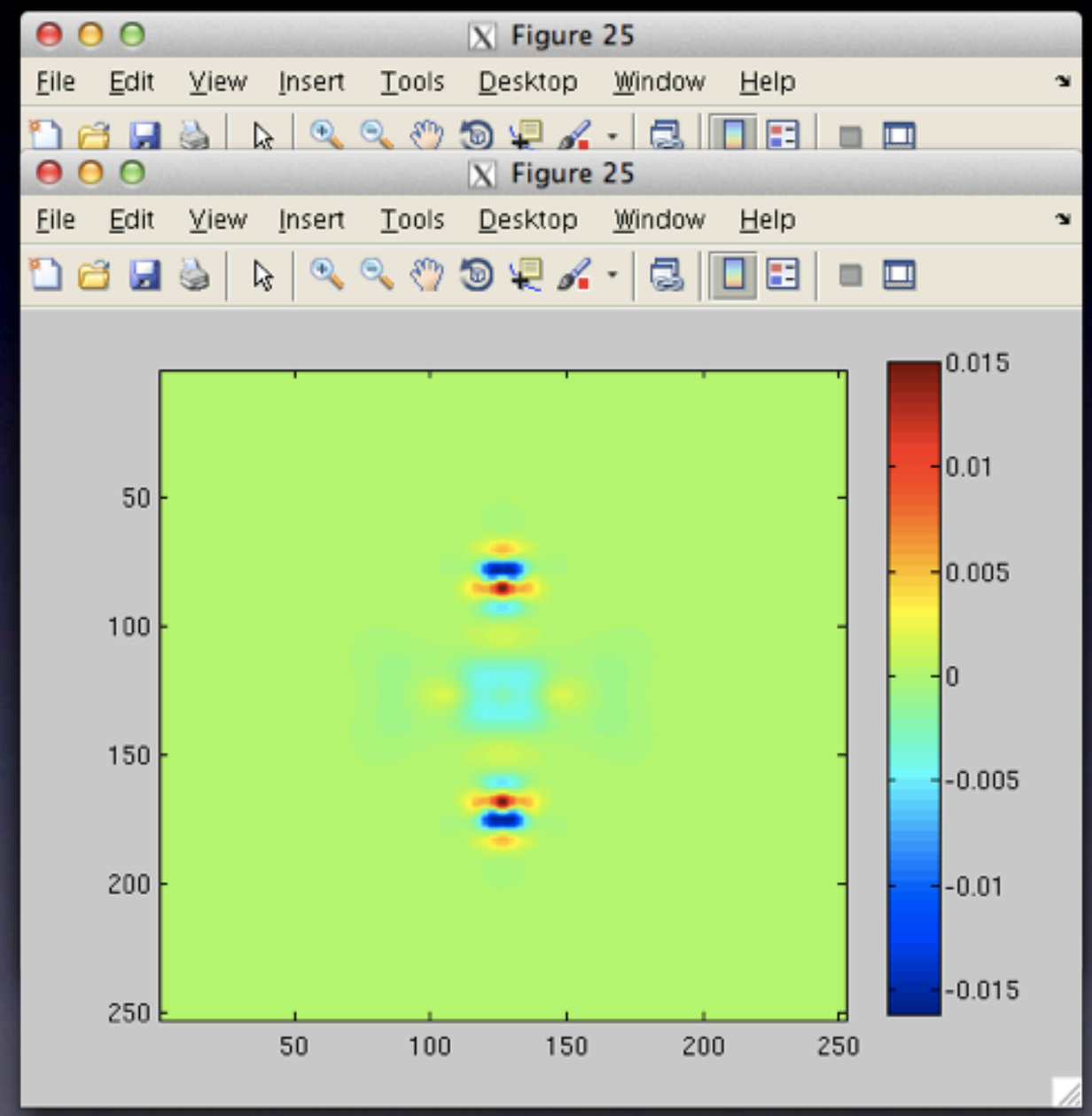
Finite Difference Method



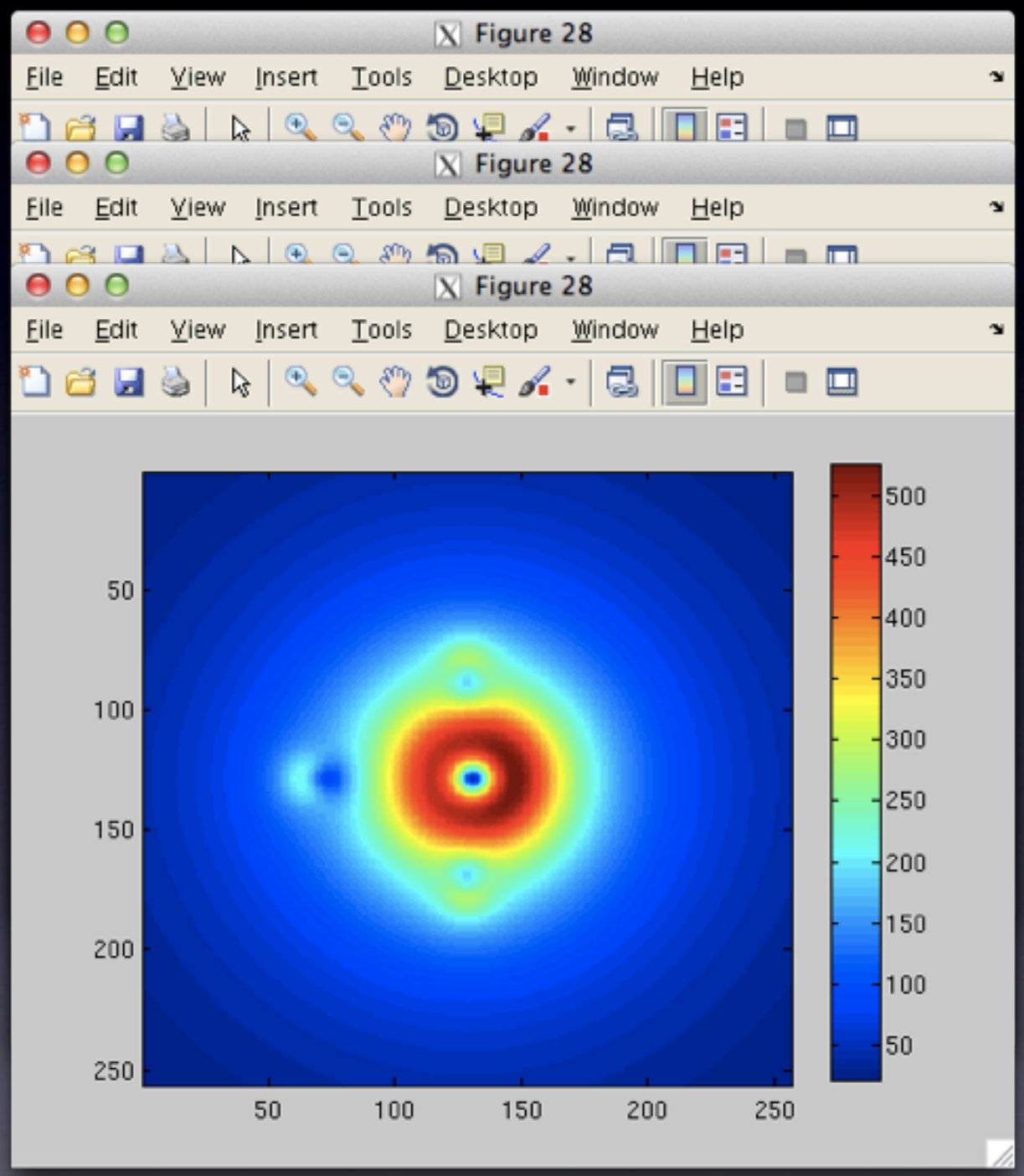


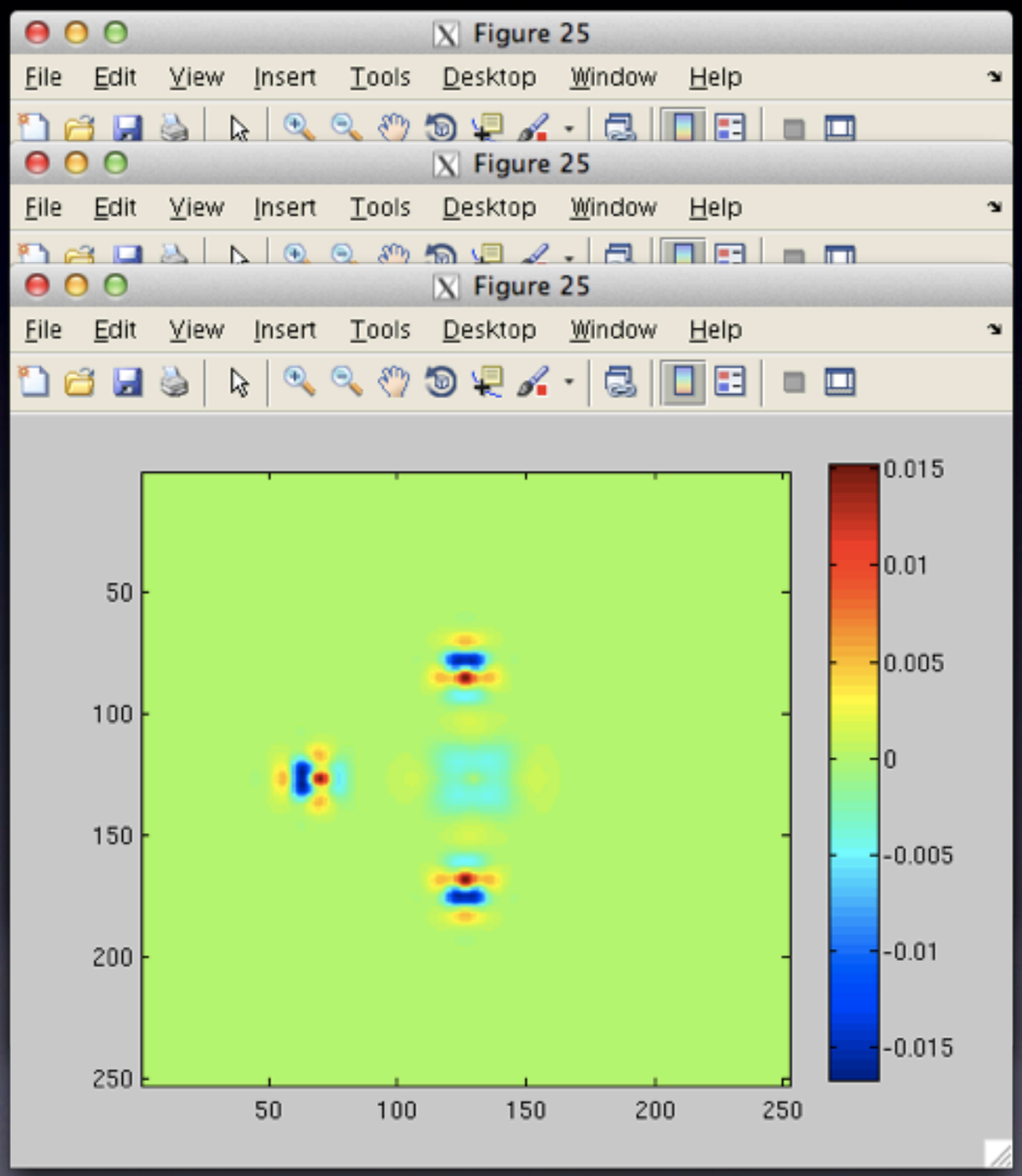
Finite Difference Method



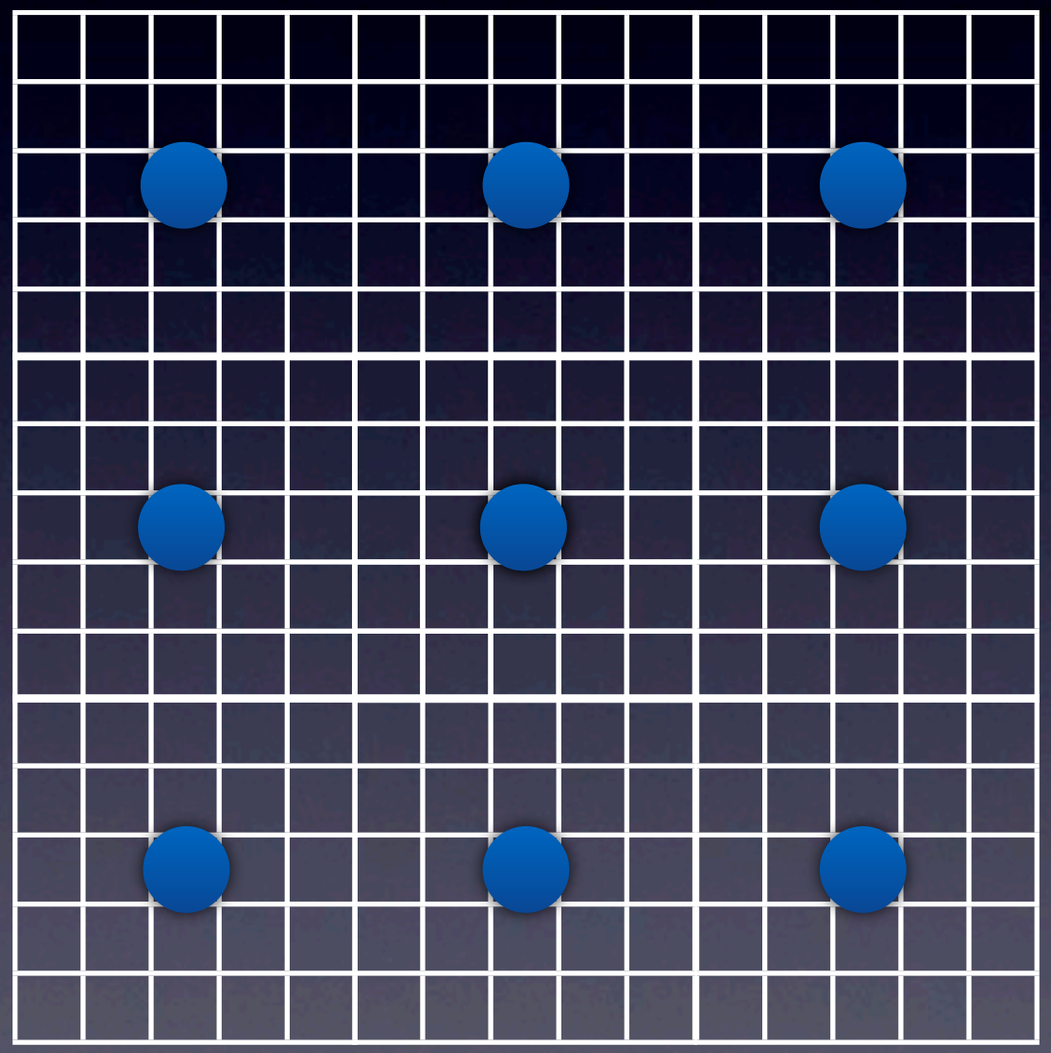


Finite Difference Method

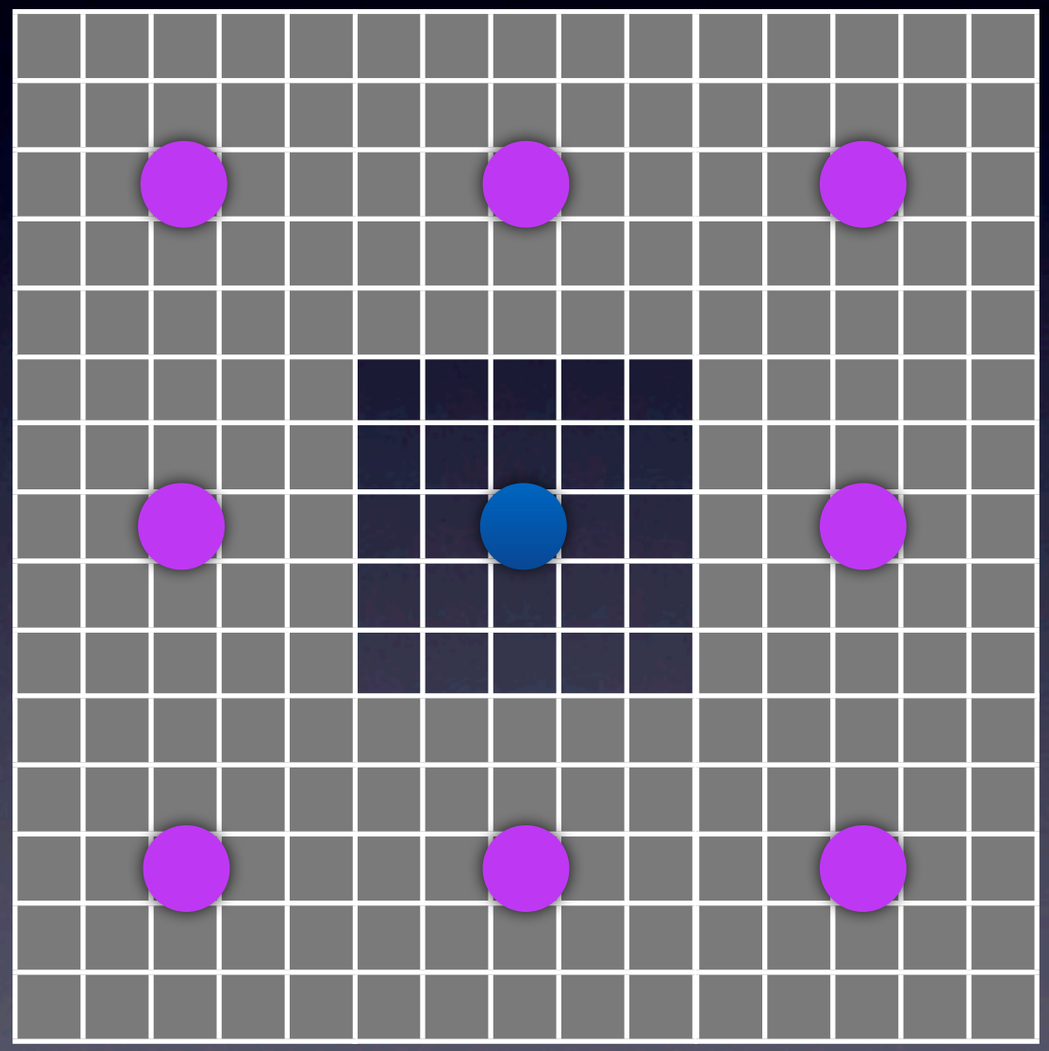




Multipole correction



Multipole correction



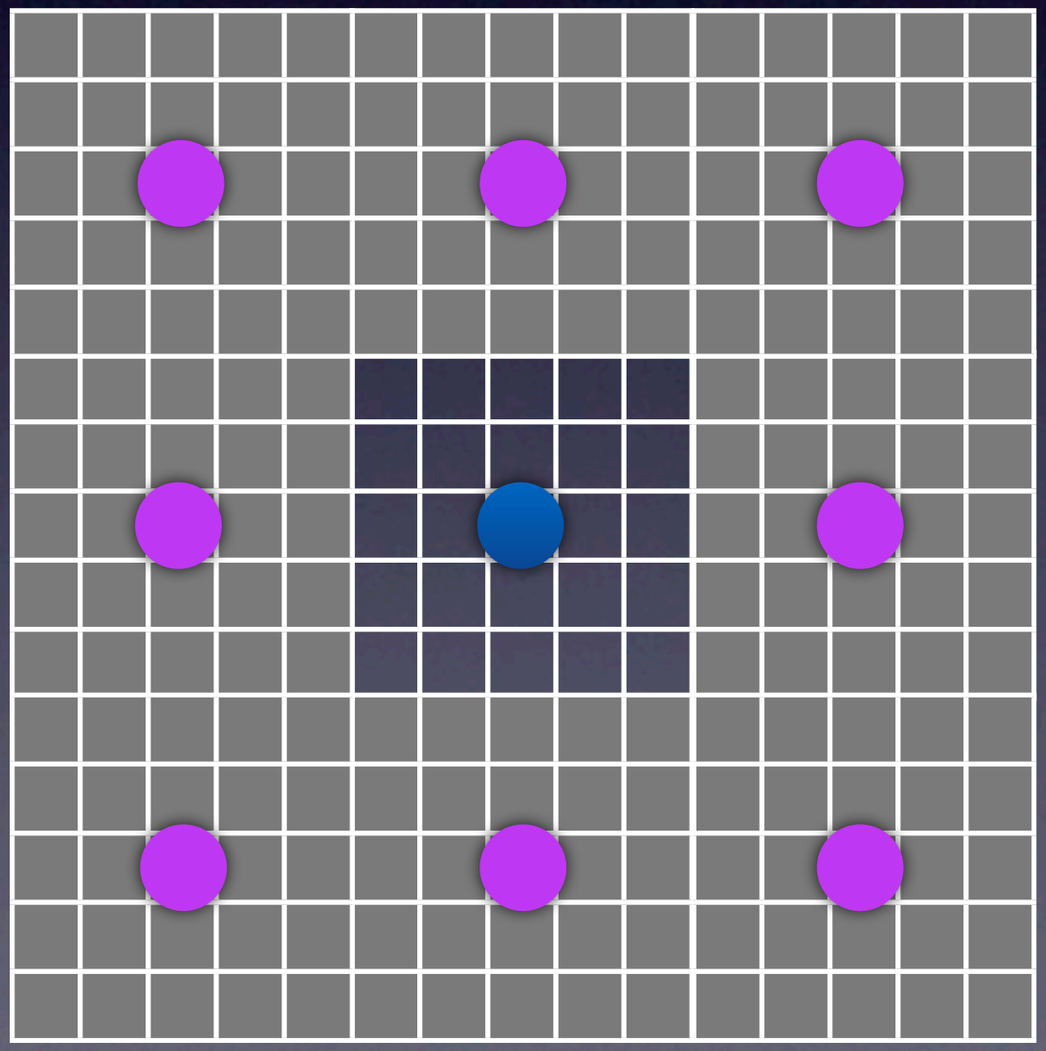
Multipole correction

$$\rho(r,\theta,\varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \rho_{lm}(r,\theta,\varphi)$$

$$\rho_{lm}(r,\theta,\varphi) = q_{lm} Y_{lm}(\theta,\varphi) f_{lm}(r)$$

$$q_{lm} = \int Y_{lm}^{*}(\theta',\varphi') r^{l} \rho(\mathbf{x}') d^{3}x'$$

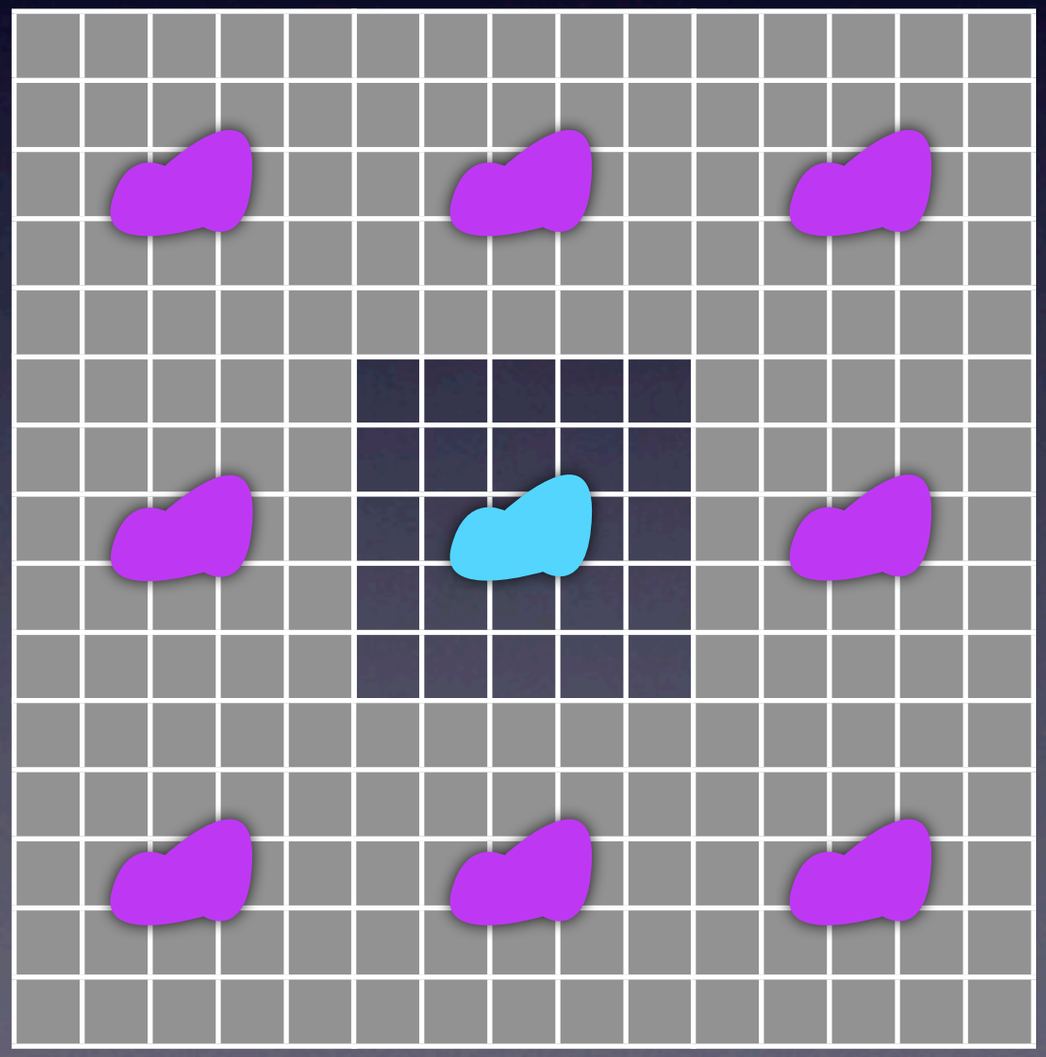
$$\nabla^{2} \phi_{lm}(\mathbf{x}) = \rho_{lm}(\mathbf{x})$$



Multipole correction

$$\phi = \phi^{\mathrm{FFT}} - \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left(\phi_{lm}^{\mathrm{FFT}} - \phi_{lm}^{\mathrm{analy}}\right)$$

$$= \phi^{\mathrm{FFT}} \begin{array}{ll} -\left(\phi_{00}^{\mathrm{FFT}} - \phi_{00}^{\mathrm{analy}}\right) & \text{monopole} \\ -\sum_{m=-1}^{1}\left(\phi_{1m}^{\mathrm{FFT}} - \phi_{1m}^{\mathrm{analy}}\right) & \text{dipole} \\ -\sum_{m=-2}^{2}\left(\phi_{2m}^{\mathrm{FFT}} - \phi_{2m}^{\mathrm{analy}}\right) & \text{quadrupole} \\ -\ldots & \text{high order term} \end{array}$$



Multipole correction

$$\phi = \phi^{\mathrm{FFT}} - \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left(\phi_{lm}^{\mathrm{FFT}} - \phi_{lm}^{\mathrm{analy}}\right)$$

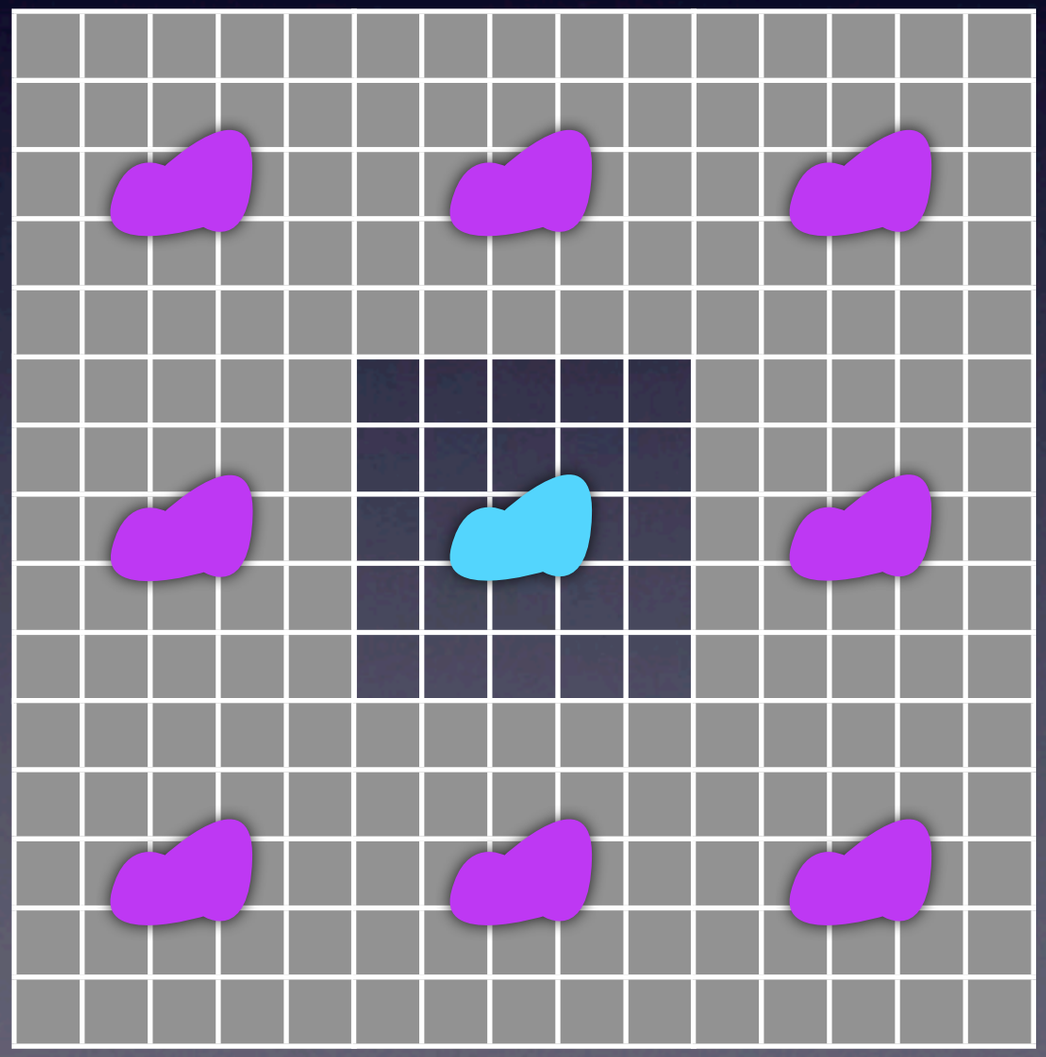
Error correct error

$$= \phi^{\mathrm{FFT}} \quad -\left(\phi_{00}^{\mathrm{FFT}} - \phi_{00}^{\mathrm{analy}}\right) \quad \text{monopole}$$

$$-\sum_{m=-1}^{1}\left(\phi_{1m}^{\mathrm{FFT}} - \phi_{1m}^{\mathrm{analy}}\right) \quad \text{dipole}$$

$$-\sum_{m=-2}^{2}\left(\phi_{2m}^{\mathrm{FFT}} - \phi_{2m}^{\mathrm{analy}}\right) \quad \text{quadrupole}$$

$$-\ldots \quad \text{high order term}$$



Multipole correction

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$$\rho_{lm}(r,\theta,\varphi) = q_{lm} Y_{lm}(\theta,\varphi) f_{lm}(r)$$

Multipole correction

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$$\rho_{00}(r) = \frac{q_{00}}{(\sigma_{00}\sqrt{2\pi})^3} \mathrm{e}^{-\frac{r^2}{2\sigma_{00}^2}} \qquad \phi_{00}(r) = -\frac{q_{00}}{4\pi r} \mathrm{erf}\left(\frac{r}{\sqrt{2}\sigma_{00}}\right) \qquad q_{00} = M_{total}$$

Multipole correction

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$$l\geq 1$$

$$f_{lm}(r)=\frac{-q_{lm}}{2l+1}\frac{(2l+1)\mathrm{e}^{-\frac{r^2}{2\sigma_{lm}^2}}(1-\mathrm{e}^{-\frac{r^2}{2\sigma_{lm}^2}})^{2l-1}}{\sigma_{lm}^2 r^{l+1}}\left[2l\frac{r^2\mathrm{e}^{-\frac{r^2}{2\sigma_{lm}^2}}}{\sigma_{lm}^2}(1-\mathrm{e}^{-\frac{r^2}{2\sigma_{lm}^2}})(2l-1+\frac{r^2}{\sigma_{lm}^2})\right]$$

Multipole correction

$$\rho(r,\theta,\varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \rho_{lm}(r,\theta,\varphi)$$

$$\rho_{lm}(r,\theta,\varphi) = q_{lm} Y_{lm}(\theta,\varphi) f_{lm}(r)$$

$$\rho_{00}(r) = \frac{q_{00}}{(\sigma_{00}\sqrt{2\pi})^3} \mathrm{e}^{-\frac{r^2}{2\sigma_{00}^2}} \qquad \phi_{00}(r) = -\frac{q_{00}}{4\pi r} \mathrm{erf}\left(\frac{r}{\sqrt{2}\sigma_{00}}\right) \qquad q_{00} = M_{total}$$

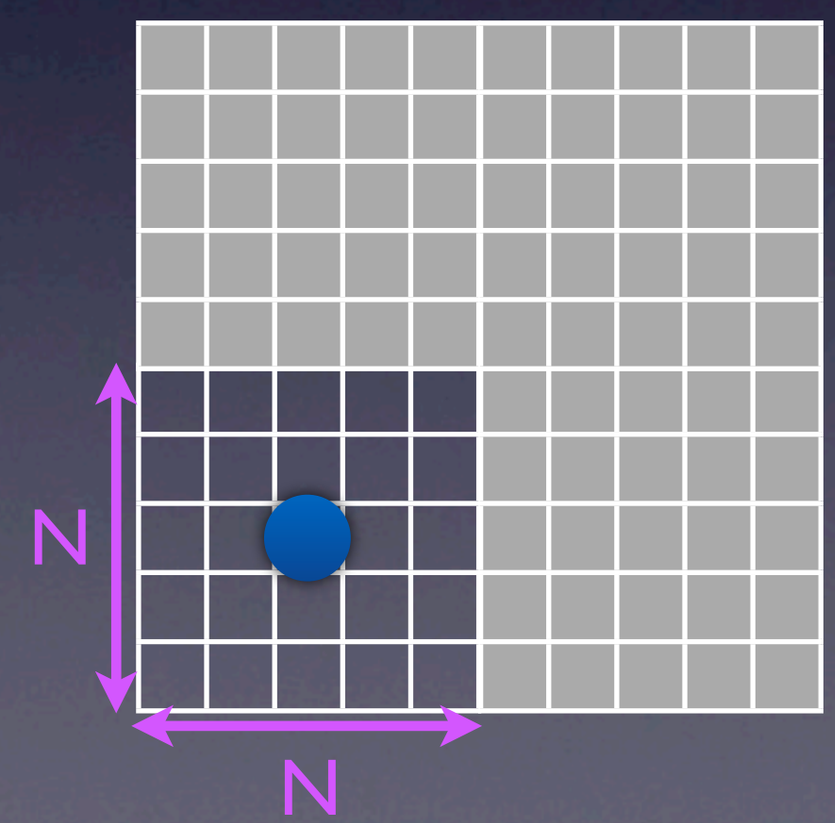
$l \geq 1$

$$\phi_{lm}(r) = \frac{(1-\mathrm{e}^{-\frac{r^2}{2\sigma_{lm}^2}})^{2l+1}}{r^{l+1}} \qquad q_{lm} = \int Y_{lm}^*(\theta',\varphi') r^l \rho(\mathbf{x}') d^3x$$

Green's Function

$$\left.\begin{aligned} G_{i,j,k} &= -\frac{1}{4\pi\sqrt{i^2+j^2+k^2}} \\ &= G_{2N-i,j,k} = G_{i,2N-j,k} = G_{i,j,2N-k} \\ &= G_{2N-i,2N-j,k} = G_{i,2N-j,2N-k} = G_{2N-i,j,2N-k} \\ &= G_{2N-i,2N-j,2N-k} \end{aligned}\right\} \begin{aligned} &0 \le i,j,k \le N \\ &i+j+k \ne 0 \end{aligned}$$

$$G_{0,0,0} = -\frac{1}{4\pi}$$



Green's Function

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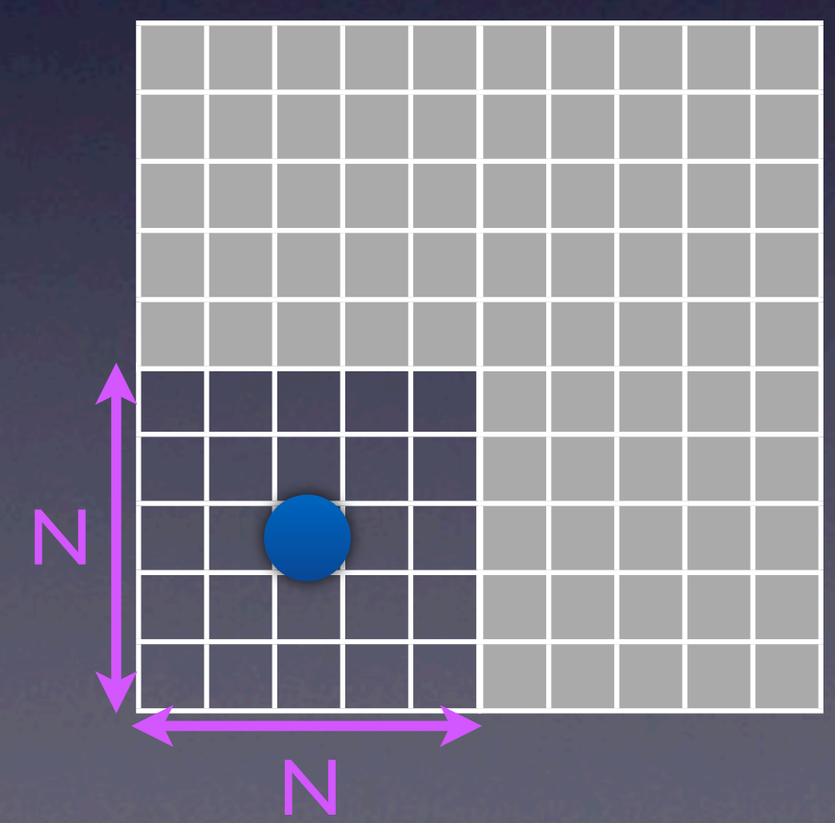

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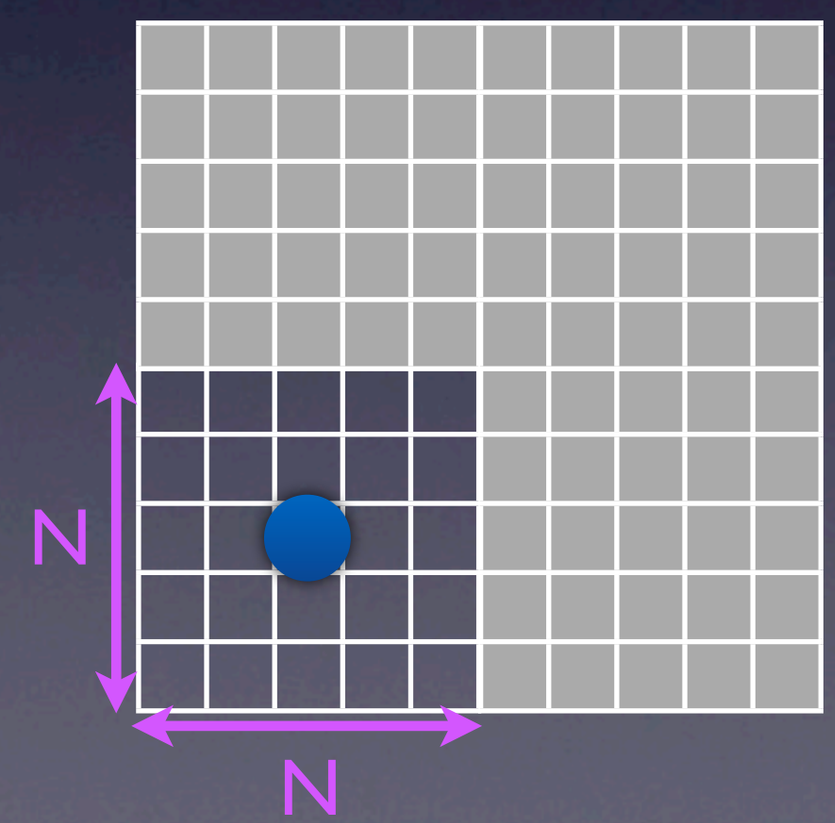
$$G_{0,0,0} = -\frac{2.8362}{4\pi}$$