程序培训-数值积分

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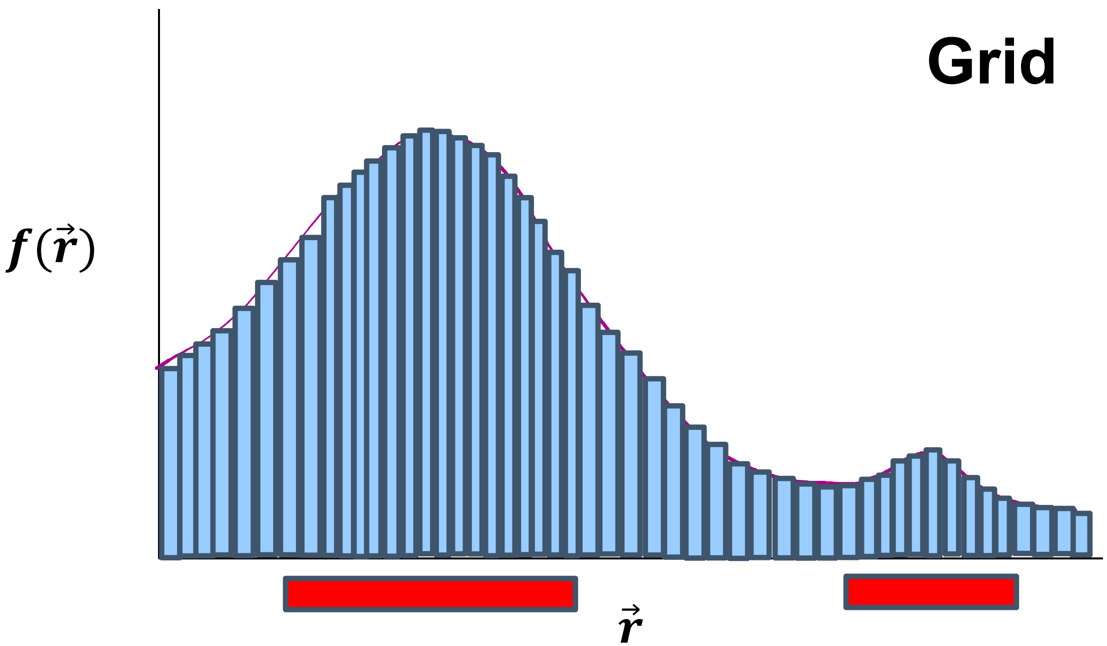
$$V = \int \boldsymbol{f}(\vec{\boldsymbol{r}})\, d\vec{\boldsymbol{r}} \quad = \sum_g \boldsymbol{f}(\vec{\boldsymbol{r}}_g)\, \boldsymbol{\omega}_g$$

Grid **Weight**



量化中什么时候需要数值积分？

$$FC = SCE$$

$$F = T + V_n + J + c_x K + F^{xc} \qquad S$$

$$\Omega_{ai} = \int |\phi_a||\phi_i| d\vec{r} \qquad D_{\mu\nu}^{\vec{r}} = < \chi_\mu | \vec{r} | \chi_\nu >$$

- 必须使用数值积分
  - **GTO**：F^{xc}，Ω_{ai}
  - **STO/ANO**：all (except 1 center STO)
- 计算加速

  MPEC-J, COSX-K, FFT-J, ……

- 产生格点
  - 均匀格点
  - 原子中心格点

- 在格点上的计算
  - 格点分块
  - 格点块上计算

均匀格点

PW，FFT-J，特殊性质

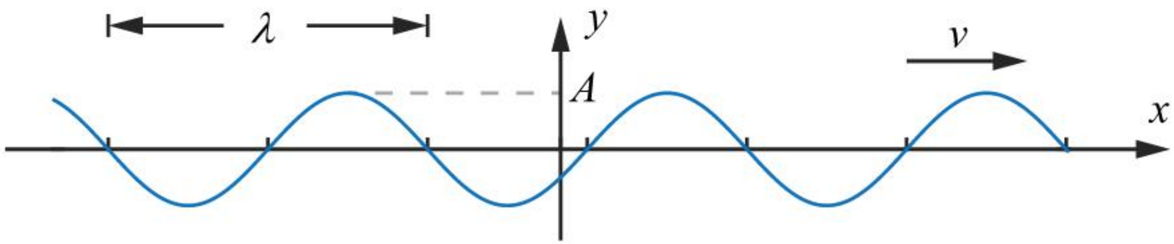
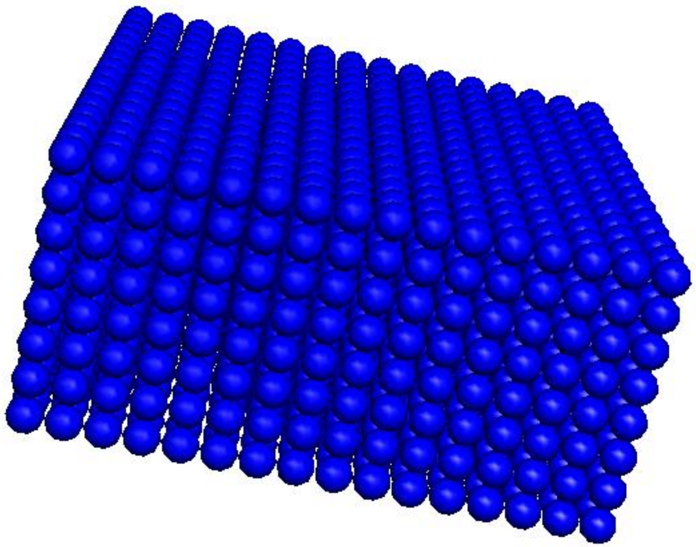
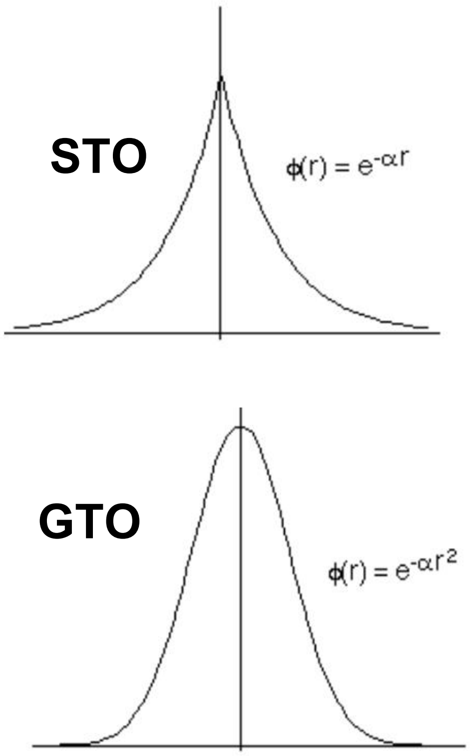


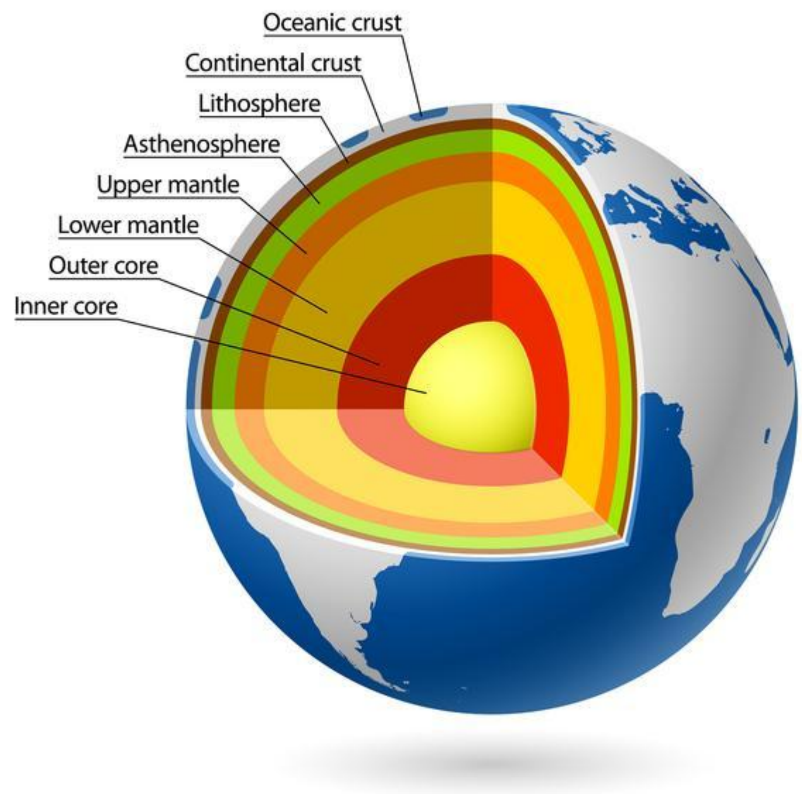
图 1：一维（平面）简谐波



原子中心格点

AO： $\chi = R(r)Y_{lm}(\theta, \phi)$ 径向×角度





原子中心格点

径向×角向

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subroutine generate_radial_grid
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"Gauss-Chebyshev "
"Gauss-Legendre "
"Multi-Exponential "
"Generalized Languerre "
"Mura-Knowles log3 "
"Murray-Handy-Laming "
"UT method "
"Euler Maclaurin "
"Second Kind Chebyshev "
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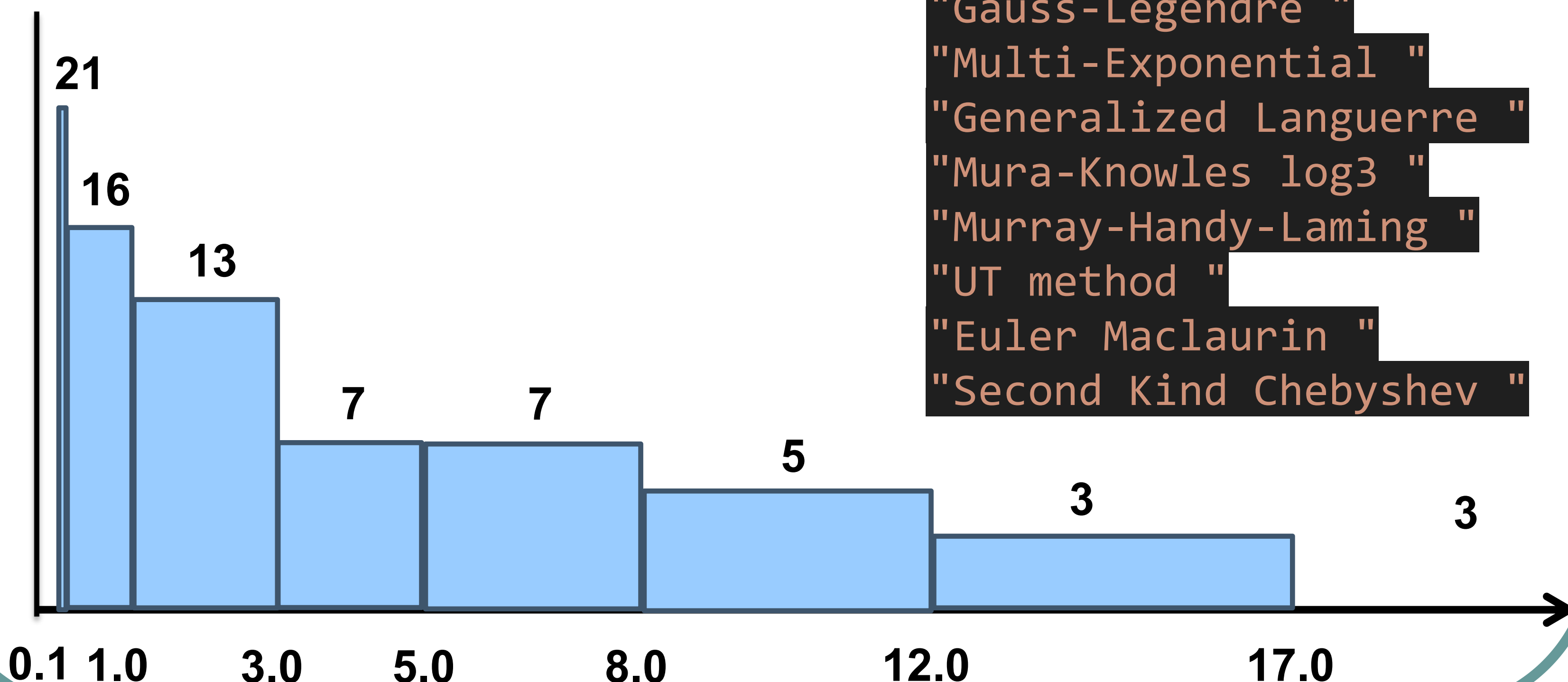
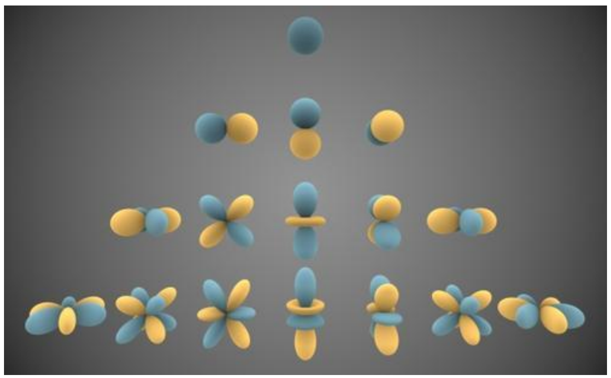


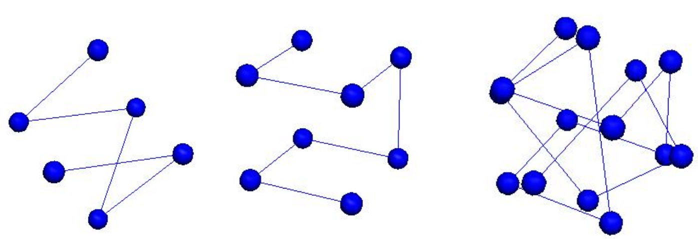
Gauss-Chebeshev used by Becke

原子中心格点

角度格点

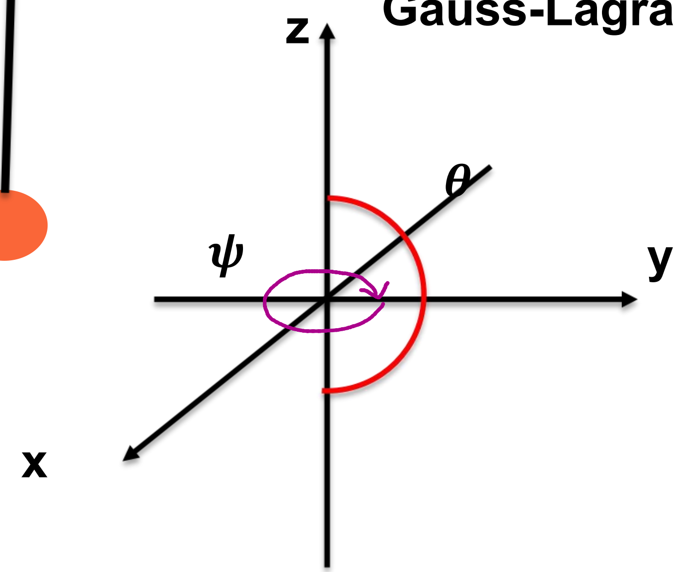


Lebedev (Oh) 5810



6 8 14

Gauss-Lagrande

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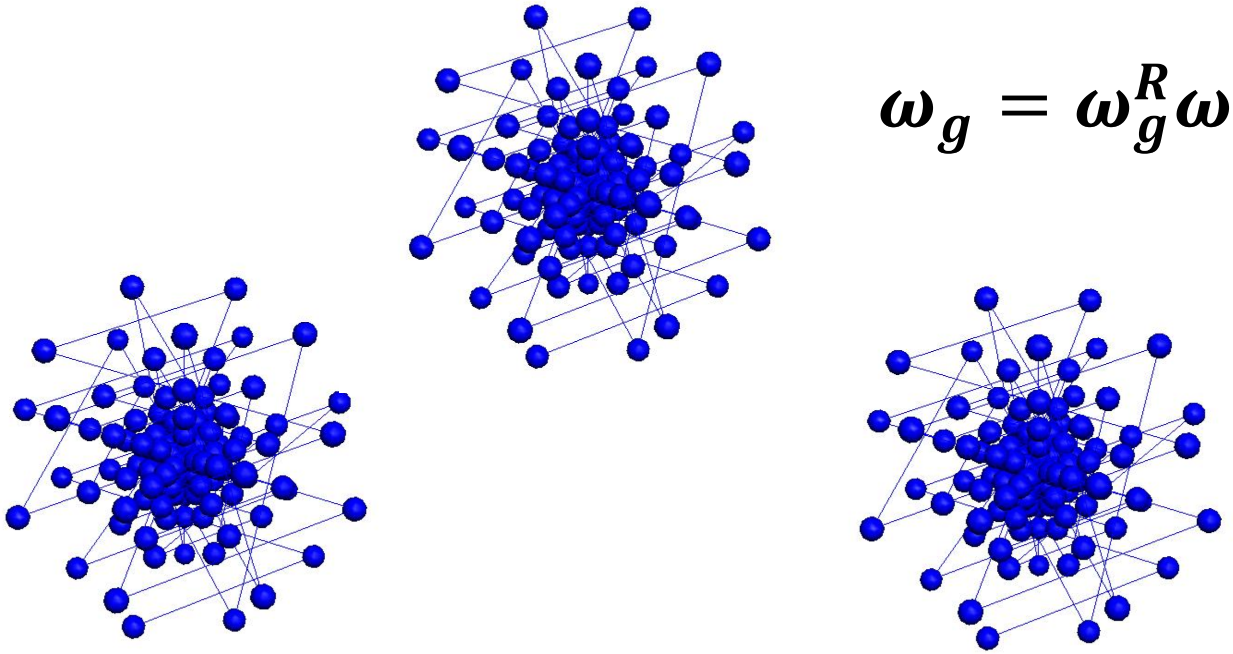
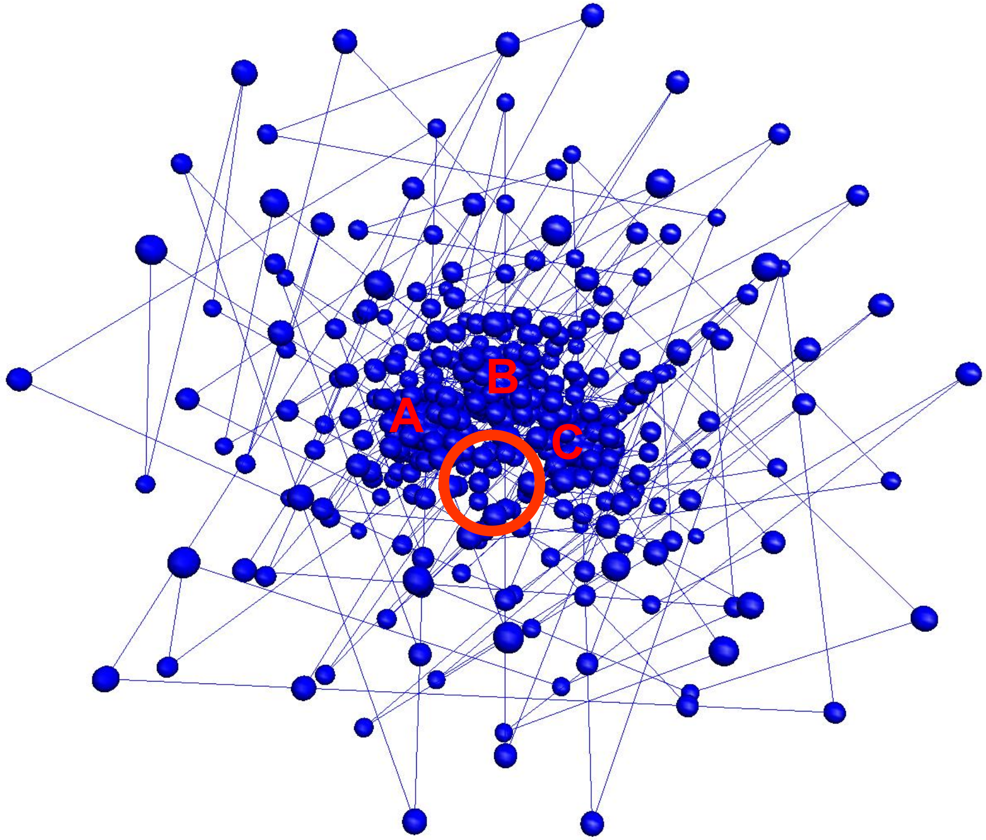
subroutine generate_angular_grid
```

径向×角度

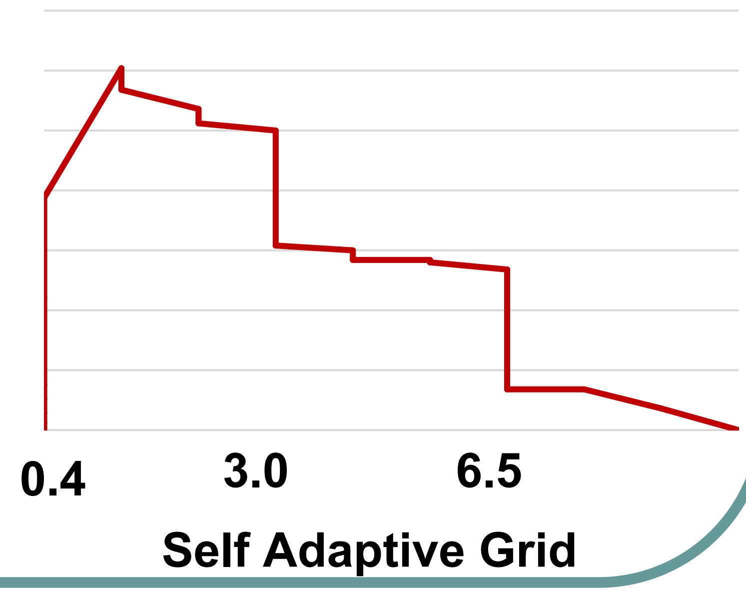


$$\omega_g = \omega_g^R \omega_g^G$$



Partition Function

$$\omega_g = \omega_g^R \omega_g^G P_A$$



Partition Function

$$\omega_g = \omega_g^R \omega_g^G P_A \qquad P_A = \frac{Q_A}{\sum_B Q_B}$$

$$Q_B = \Pi_{C \neq B} F_{CB} \qquad Q_B = \rho_B^2(r_g)$$ Delley

$$F_{CB} = \frac{1}{2} - \frac{1}{2} f(u_{CB}), \;\; u_{CB} = \frac{|r_g - R_B| - |r_g - R_C|}{|R_B - R_C|}$$

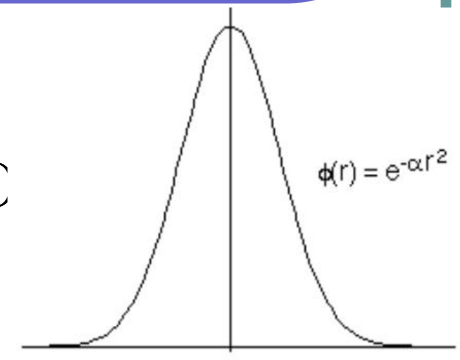
$$f(u) = g\left(g(g(u))\right), \; g(u) = \frac{3}{2}u - \frac{1}{2}u^3$$ **Becke**

$$f(u) = \begin{cases} -1 & u \in (-\infty, \; -0.64] \\ \frac{-5u^7+21u^5-35u^3+35u}{16} & u \in (-0.64, +0.64) \\ +1 & u \in (+0.64, \; +\infty] \end{cases}$$ **SSF**

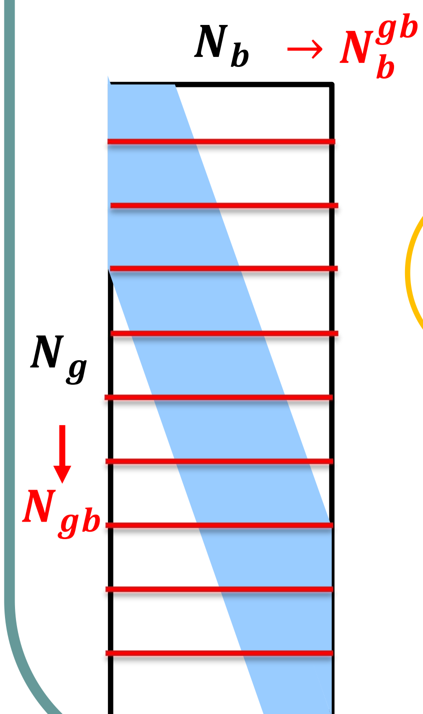
在格点上的计算：基组，分块

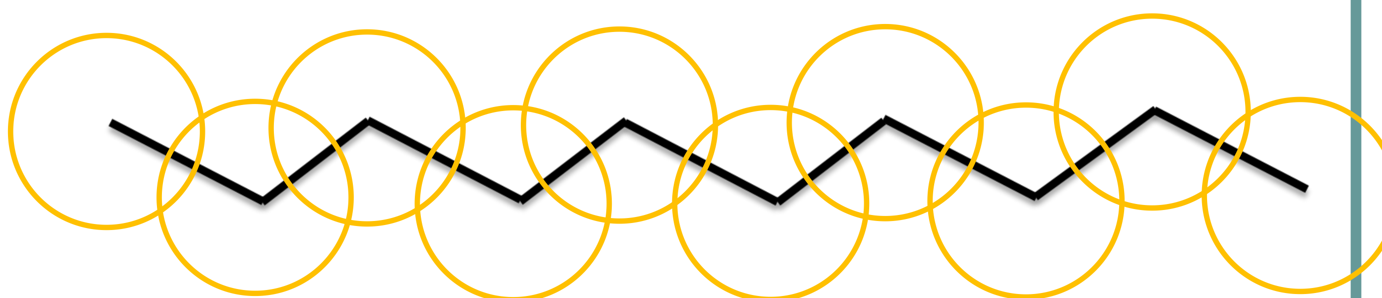
格点上的基组计算：

$$\chi(\vec{r}, \vec{R}, \alpha, l, m) = O_{\alpha l m} r^{l} e^{-\alpha r^2} Y_{lm}(\theta, \varphi)$$



$$f(R_{\mu}^{cut}) = \int_{R_{\mu}^{cut}}^{\infty} Q_{\mu}^{2}(r) 4\pi r^2 dr = 10^{-\eta}$$





"稀疏矩阵"

Storage, Cache…

Grid Batch (128)

在格点上的计算

格点上的电子密度

$$\rho(r_g) = \sum \underbrace{D_{\nu\mu}\chi_\mu(r_g)}_{\boldsymbol{a_\nu(r_g)}}\chi_\nu(r_g)$$

$$\boldsymbol{N_g \times 2 \times N_b \times N_b}$$

$$\boldsymbol{N_g \times N_b \times (N_b + 1)}$$

$$\boldsymbol{N_{gb} \times 128 \times N_b^{gb} \times (N_b^{gb} + 1)}$$

思考：$\nabla\rho(r_g) = \sum D_{\nu\mu}\nabla(\chi_\mu(r_g)\chi_\nu(r_g))$

在格点上的计算

$\boldsymbol{GGA}$的交换相关矩阵$\boldsymbol{F_{\mu\nu}^{xc}}$构造

$$F_{\mu\nu}^{xc} = < \chi_\mu | \frac{\delta E_{xc}}{\delta \rho} | \chi_\nu >$$

$$\boldsymbol{N_g \times 12 \times N_b \times N_b}$$

$$= \int dr \{ \chi_\mu^\dagger \frac{\partial E_{xc}}{\partial \rho(r)} \chi_\nu + \frac{\partial E_{xc}}{\partial \nabla \rho(r)} \cdot (\chi_\mu^\dagger \nabla \chi_\nu + \chi_\nu \nabla \chi_\mu^\dagger)\}$$

$$= \sum\nolimits_{\boldsymbol{r_g}} \omega_g \{ \chi_\mu^\dagger(r_g) \chi_\nu(r_g) V_{xc}(r_g)$$

$$+ V_{xc}^{\nabla}(r_g) \cdot (\chi_\mu^\dagger(\boldsymbol{r_g}) \nabla \chi_\nu(\boldsymbol{r_g}) + \chi_\nu(\boldsymbol{r_g}) \nabla \chi_\mu^\dagger(\boldsymbol{r_g}))\}$$

在格点上的计算

$\boldsymbol{GGA}$的交换相关矩阵$\boldsymbol{F_{\mu\nu}^{xc}}$构造

- 直接实现$F_{\mu\nu}^{xc}$的计算程序 $\boldsymbol{N_g \times 12 \times N_b \times N_b}$

- 如何提高效率？
  - 基组局域性, grid batch
  - 算法：构造中间量，对称性，矩阵乘
  - 使用高效的矩阵乘程序：MKL::dgemm

Thanks